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GROUNDWATER MODELS: A COMPARISON USING FIELD DATA

M. KOLODNY

DYNAMAC CORPORATION
1140 ROCKVILLE PIKE
ROCKVILLE MD 20852

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TYNDALL AIR FORCE BASE, FLORIDA 32403

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This report evaluates the simulation capabilities of three groundwater transport computer models. The models evaluated were: (1) Saturated-Unsaturated Transport SUTRA; (2) Random Walk Solute Transport; and (3) the US Geological Survey Two-Dimensional Solute Transport and Dispersion. The models were compared on their input data requirements, ease of use, computer time, limitations, flexibility, readability of results, and accuracy. Field data were compared to model results. Our evaluations showed that no major differences between the simulation results of the USGS-2D and Random Walk Models. The SUTRA program was not adequately tested, so no definitive statements can be made for this computer model.

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PREFACE

This report was prepared by Dynamac Corporation, 11140 Rockville Pike, Rockville, Maryland 20852, under contract number F08635-85-C-0057, for Air Force Engineering and Services Center, Engineering and Services Laboratory (HQ AFESC/RDVW), Tyndall Air Force Base, Florida 32403-6001. The project officer was Captain Edward Heyse.

This report evaluates the simulation capabilities of three groundwater transport computer models. The models evaluated are: (1) Saturated-Unsaturated Transport SUTRA, (2) Random Walk Solute Transport, and (3) the U.S. Geological Survey Two-Dimensional Solute Transport and Dispersion. The study was performed between 28 June 1985 and 15 May 1988.

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This report has been reviewed by the Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication.

Michael G. Elliott

MICHAEL G. ELLIOTT, 1Lt, USAF, BSC
Environmental Research Engineer

Nils Akerlind Jr.

NILS AKERLIND, JR., Major, USAF
Chief, Environics Division

F. THOMAS LUBOZYNSKI, Major, USAF, BSC
Chief, Environmental Engineering Branch

LAWRENCE D. HOKANSON, Colonel, USAF
Director, Engineering and Services Laboratory

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SECTION I

INTRODUCTION

A. OBJECTIVE

The objective of this project was to test and evaluate three groundwater solute transport models available for running on the Air Force Engineering and Services Center (AFESC) computer. These tests and evaluations were conducted to: (1) identify problems involved with modeling real-field data on AFESC hardware; (2) compare the simulation accuracy and the relative benefits and limitations of the three models; and (3) test the sensitivity of various input parameters. The ultimate goal was to recommend research needs and technology transfer opportunities in groundwater modeling for the Air Force Installation Restoration Program (IRP).

B. BACKGROUND

Computer models can support IRP and similar remedial assessments and implementations. For example, groundwater solute modeling has been used to help determine the extent of contaminant migration in the aquifers beneath Wurtsmith AFB, Michigan (Reference 1) and Air Force Plant 44, Tucson, Arizona (Reference 2).

AFESC has three groundwater solute transport models on the Center's CDC CYBER 170/130 computer.

1. USGS-2D

A two-dimensional, groundwater solute transport model using an alternating-direction implicit procedure to solve the finite-difference approximation of the groundwater flow equation, and the method of characteristics to solve the solute transport equation (References 3, 4).

2. Illinois Random Walk Model

A two-dimensional, groundwater solute transport model using a modified iterative alternating-direction implicit procedure to solve the finite difference approximation of the groundwater flow equation, a particle-in-a-cell technique for the convective mechanisms in the solute transport equation, and a random walk technique for the dispersion effects (References 5, 6).

3. SUTRA Model

A two-dimensional hybrid finite-element and integrated-finite-difference method to approximate the governing equations that describe the following interdependent processes:

a. Fluid density-dependent saturated or unsaturated groundwater flow, and either,

b. Transport of a solute in the groundwater or,

c. Transport of thermal energy in the groundwater and the solid matrix of the aquifer.

AFESC cofunded development of the SUTRA model (References 7, 8).

Before investing further in groundwater modeling, AFESC decided to test and compare the three models using Air Force field data. The results of this study will help AFESC to decide how to proceed with groundwater modeling research.

C. SCOPE

This effort consisted of the following tasks:

1. Update Models

The three models were updated as appropriate and prepared to run on the AFESC computer.

2. Data Collection and Integration

An Air Force groundwater pollution site was chosen to adequately test the various capabilities of the three models.

3. Model Calibration

The models were calibrated for the selected site. Data requirements for each model were documented and the sensitivity of model parameters for site-specific application was demonstrated.

4. Evaluation of Models

The calibrated models were run to test the following capabilities:

a. Model accuracy with reference to known sample problems.

b. Model prediction of the extent of pollutant plumes in groundwater systems.

c. Model discrimination between the fates of conservative contaminants and contaminants influenced by chemical reactions, degradation, and adsorption.

5. Model Comparison

The relative advantages and disadvantages of each model were assessed as follows:

a. Data requirements.

b. Model sophistication.

c. Model accuracy.

d. Readability of simulation results.

e. Computation time and memory requirements.

f. Overall cost factors.

6. Modeling Recommendations

Research needs and information concerning groundwater modeling to support the Air Force IRP were identified.

SECTION II

THE USGS-2D MODEL

The USGS-2D (Konikow and Bredehoeft) program is a finite-difference model for groundwater flow, coupled with a method of characteristics model for solute transport (Reference 3). This United States Geological Survey (USGS) model, published in 1978, features a two-dimensional, areal, rectangular grid for simulating a conservative solute. A revised program for a nonconservative solute was written in 1982 (Reference 4) to include radioactive decay, adsorption, and chemical reaction effects on solute transport. For steady-state groundwater flow, the flow routine and the solute transport routine can be uncoupled and solved sequentially.

A. FLOW ROUTINE

The groundwater flow routine is based on several major assumptions. The program is normally used for two-dimensional (2-D) areal simulations, though it can be adapted for vertical cross-section simulations. An Alternating Direction Implicit Procedure (ADIP) is used to numerically solve the governing equations.

1. Governing Equations

Water flows are assumed to follow Darcy's Law:

$$V_i = - \frac{K_{ij}}{\varepsilon} \frac{\partial h}{\partial x_j} \qquad (1)$$

where the right-hand side is summed over the two rectangular coordinates $j = 1,2$, and where:

V = seepage, or average velocity of water in the pores (ft/sec),

K_{ij} = hydraulic conductivity (ft/sec),

h = hydraulic head (ft), and

ε = aquifer porosity (volume fraction).

No variations are assumed in the vertical direction, except that:

- cell thickness may vary cellwise, and
- leakage occurs vertically between aquifers (or strata).

The differential equation for the head difference in the groundwater flow field is (Reference 3):

$$\frac{\partial}{\partial x_i}\left[T_{ij}\frac{\partial h}{\partial x_j}\right] = S\frac{\partial h}{\partial t} + W \qquad (2)$$

(flow) (accumulation) (source/sink)

where the left side of the equation is summed over i, j = 1,2 and where:

T_{ij} = the transmissivity tensor (ft^2/sec)

S = storativity (dimensionless),

t = time (sec), and

W = W(x,y,t) = source term (ft/sec) (+ = outflow).

The source term can be expressed as:

$$W(x,y,t) = Q(x,y,t) - \frac{K_z}{b}(H_s - h) \qquad (3)$$

where:

Q = diffuse withdrawal/recharge rate (ft/sec),

K_z = mean vertical *hydraulic conductivity* of confining layer (ft/sec),

b = thickness of the confining layer (ft), and

H_s = the hydraulic head for the source stream (ft).

The above differential equations are converted into finite-difference form for numerical solution. The difference equations are detailed on pages 8-11 of the user's manual (Reference 3).

2. Numerical Solution

A number of requirements exist for setting up the solution grid which is composed of rectangular cells of uniform length and width. The nodes are located at the centers of the cells. The computer program assumes that the outermost row (or column) at each edge of the grid is always comprised of impermeable cells of zero thickness. Zero thickness indicates to the ADIP that a cell is not part of the aquifer. Failure to specify zero thicknesses at the edges of the grid leads to fatal execution time errors. When modeling only a portion of an aquifer, all sources and/or sinks that affect the modeled area from outside must be relocated to within the impermeable boundary. If the aquifer's domain of computation is not rectangular, an oversize grid with impermeable cells outside of the permeable portion of the aquifer is used (Figure 1).

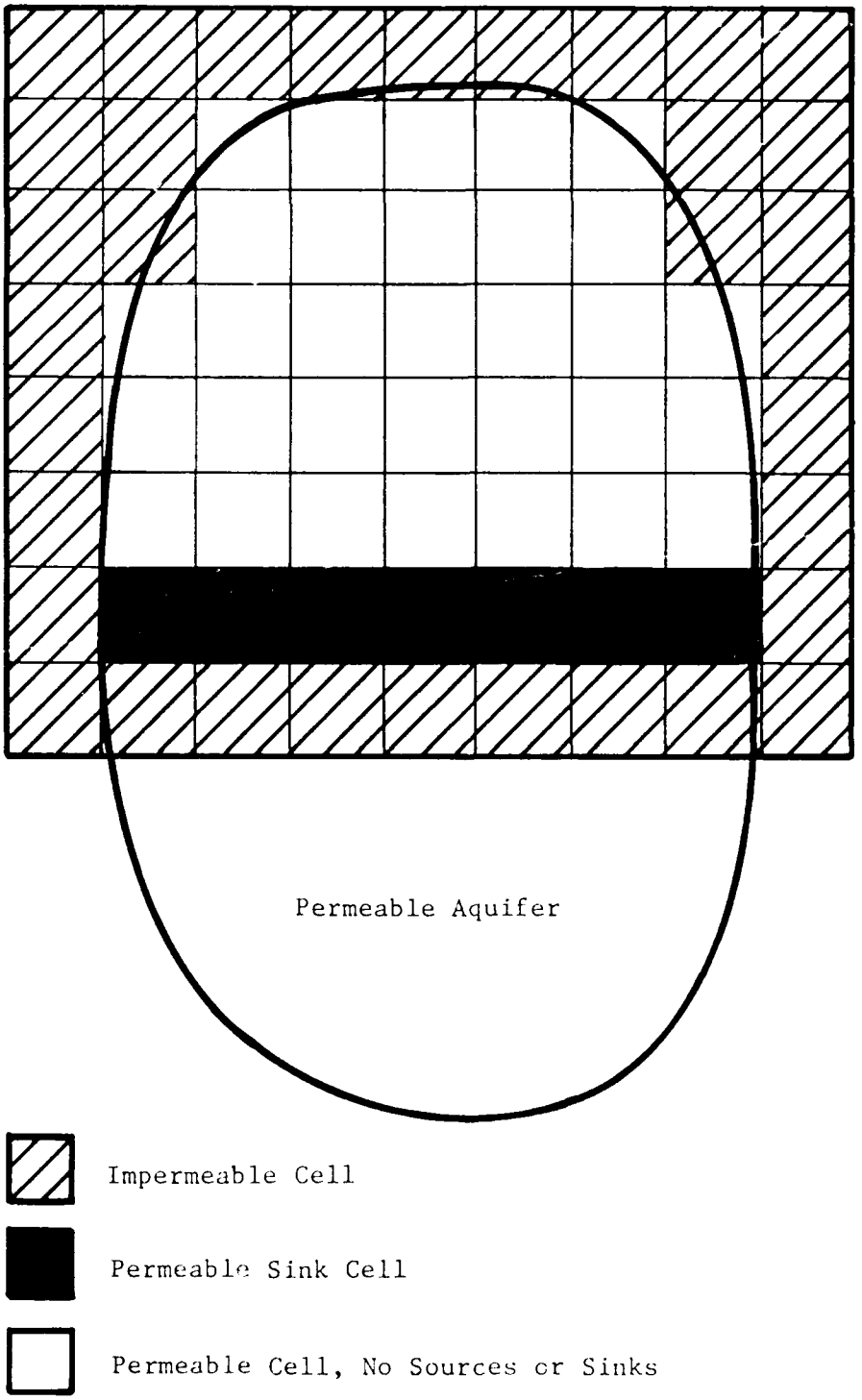


Figure 1. Setting Up a Grid for the USGS-2D Model.

The following aquifer parameters are treated as uniform over time and over the permeable cells:

- porosity (POROS)
- storage coefficient (S)
- longitudinal dispersivity (BETA)
- tranverse dispersivity (BETA)(DLTRAT)
- anisotropy (ANFCTR) (ratio of Tyy/Txx and Kyy/Kxx)

The following fluid properties (not explicit parameters) are treated as uniform over time and over the permeable cells, and uniform with respect to composition:

- temperature
- viscosity
- density

The following properties are specified by cell and treated as uniform over time:

- transmissivity (T/(I,J))
- diffuse recharge rate (head-independant) (RECH(I,J))
- leaky artesian boundary condition, "leakance" (CNRECH(I,J))
- saturated cell thickness (THCK(I,J))
- constant-head boundary conditions (WT(I,J)).

B. SOLUTE TRANSPORT

1. Governing Equation

The differential equation for solute transport is (Reference 3):

$$\underset{\text{(accumulation)}}{\frac{\partial}{\partial t}(C\,b)} = \underset{\text{(dispersion)}}{\frac{\partial}{\partial x_i}\left[b\,D_{ij}\,\frac{\partial C}{\partial x_j} \right]} - \underset{\text{(advection)}}{\frac{\partial}{\partial x_i}\left[b\,C\,V_i \right]} - \underset{\text{(source/sink)}}{\frac{C'W}{\varepsilon}}, \quad i,j = 1,2 \qquad (4)$$

where:

C = concentration of the solute (ppm),

D_{ij} = tensor coefficients of hydrodynamic dispersion (ft^2/sec),

b = aquifer cell saturated thickness (ft), and

C' = concentration of dissolved chemical in source fluid (ppm).

This differential equation is solved numerically. The user's manual (Reference 3) gives the corresponding finite-difference form of the system.

The dispersion coefficients in terms of (x,y)-coordinates are given by

$$D_{xx} = D_L(V_x)^2/|V| + D_T(V_y)^2/|V|$$

$$D_{yy} = D_T(V_x)^2/|V| + D_L(V_y)^2/|V| \qquad (5)$$

$$D_{xy} = D_{yx} = \left(D_L - D_T\right) V_x V_y /|V|^2$$

The longitudinal dispersion coefficient, DL, is defined as:

$$D_L = \alpha_L |V| \quad (ft^2/sec) \qquad (6)$$

where:

α_L = mean longitudinal dispersivity of the aquifer matrix [ft], and

$$|V| = \left(V_x^2 + V_y^2\right)^{1/2} \quad (ft/sec)$$

The transverse dispersivity coefficient, D_T, is defined as:

$$D_T = \alpha_T |V| \quad (ft^2/sec) \qquad (7)$$

where:

α_T = the mean transverse dispersivity of the aquifer matrix (ft).

In this program:

$$\alpha_T = \alpha_L \text{ (DLTRAT)}$$

where: DLTRAT is an input parameter.

2. Numerical Solution

Solute transport is simulated by the Method of Characteristics (MOC). MOC works best for hyperbolic differential equations, which apply in

groundwater modeling cases when advection is the most dominant solute transport mechanism (Reference 3). This method invokes the following major assumptions:

- Groundwater and solute transport are represented by "particles."
- Each particle has a variable solute concentration.
- The analytical frame of reference moves with the particles.
- The particle paths approximate the streamlines within the velocity field.

Particle paths do not coincide with the streamlines due to numerical approximations. A particle's velocity is calculated at the start of each time period, and it maintains this velocity for the duration of its move (Figure 2). The velocity is estimated by a four-point interpolation method at the beginning of each time period (Figure 3). The length of each time period is set by a built-in logic to maintain the algorithm's mathematical stability.

The program calculates three MOC stability criteria (Reference 3) for each particle at the start of every time period to set the length of that time period. The criteria are:

$$\Delta t \leq 0.5 \left[\frac{D_{xx}}{(\Delta x)^2} + \frac{D_{yy}}{(\Delta y)^2} \right]^{-1} \qquad (8)$$

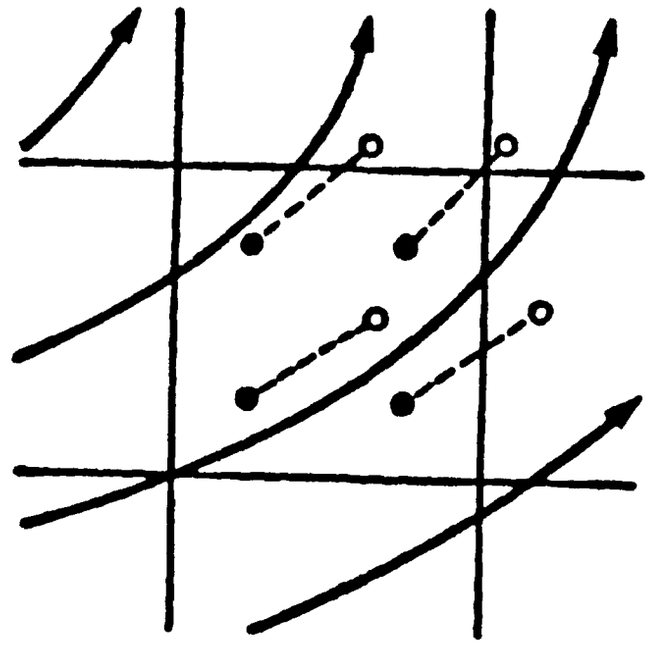
- A cell cannot be flushed out more than once per time period by an external fluid source.
- A particle cannot move a distance more than a user-specified fraction (CELDIS) of a cell length (or width) before its velocity is reinterpolated.

The duration of a particle's move-period (Δt) is determined each time the velocity field changes. This period is calculated to satisfy the three stability criteria for each cell, and the shortest of all calculated durations is chosen to apply for all cells.

Other major assumptions of the USGS-2D model include:

- perfect vertical mixing (no vertical concentration gradients exist).
- no solute exchange between aquifers and surface waters contained in ponds and lakes.

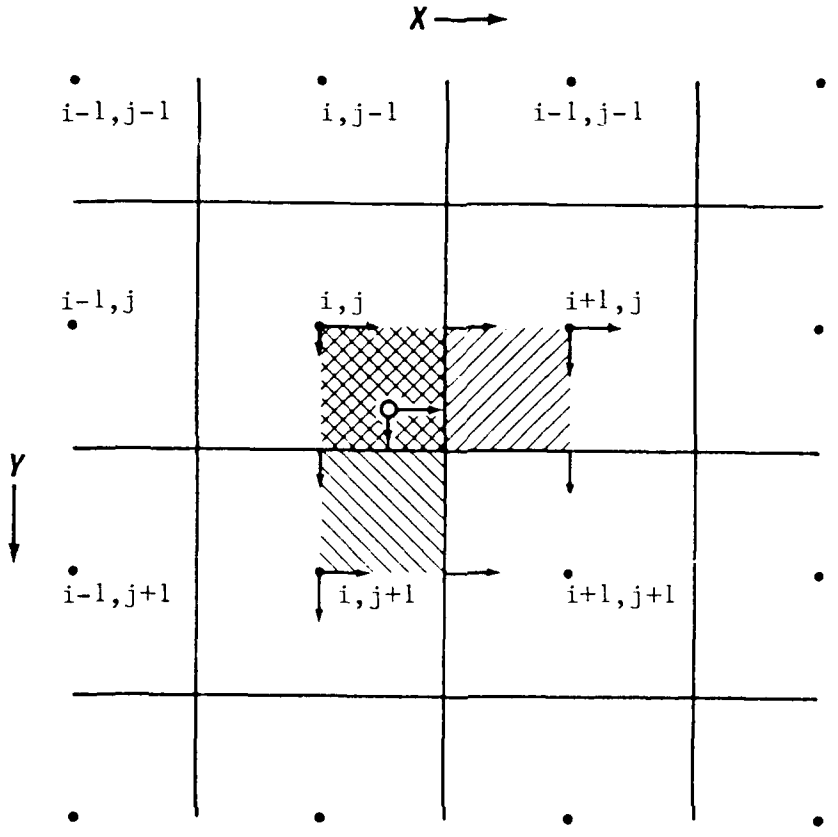
The user can control the number of particles used in this simulation (Reference 3). The initial distribution of particles is uniform, and the input parameter NPTPND specifies 4, 5, 8 or 9 particles per cell (Figure 4). A coding option allows 16 particles per cell, but this option would exceed the



EXPLANATION

•	Initial location of particle
°	New location of particle
→	Flow line and direction of flow
---	Computed path of particle

Figure 2. Relation of Flow Field to Movement of Points (Reference 3).



EXPLANATION

- • Node of finite-difference grid
- ° Location of particle p
- → X or Y component of velocity
- Area of influence for interpolating velocity in X direction at particle p
- Area of influence for interpolating velocity in Y direction at particle p

NOTE: Each area of influence is equal to one-half of the area of a cell.

Figure 3. Schematic of Bilinear Interpolation of Velocity of a Particle (Reference 3).

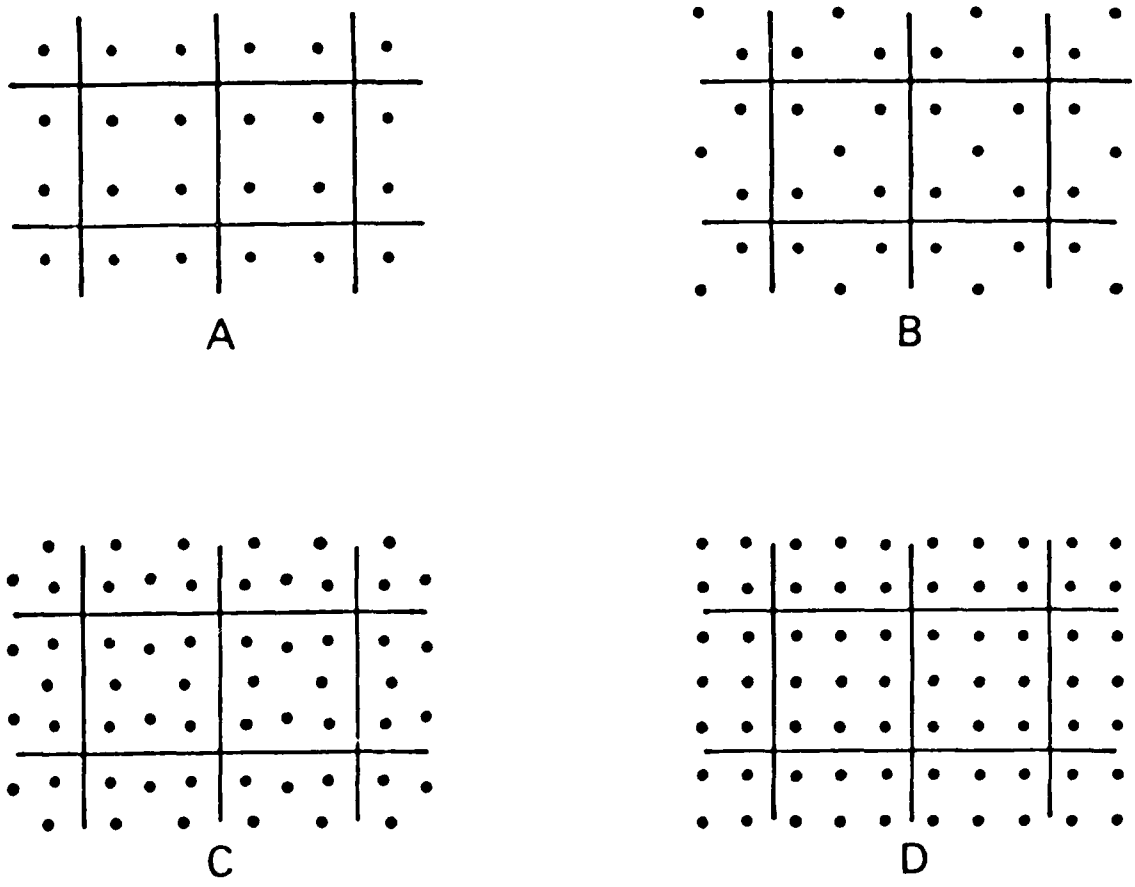


Figure 4. Geometry of Particle Distribution for Four (A), Five (B), Eight (C), and Nine (D) Particles Per Cell (Reference 3).

CYBER system's core limitations in many cases. Because the particles represent groundwater, not pure solute, the number of particles stays relatively constant during simulations with steady-state flow and conservative solute.

The simulation of one particle movement period requires several steps:

- Recalculate the length of the time period, when necessary, using the program's mathematical stability criteria.
- Calculate the effects of dispersion, divergence of velocity, sources and sinks, and changes in saturated thickness. Temporarily store the results, but do not change particle locations or concentrations yet.
- Now move the particles by advection only.
- Recalculate the effects of dispersion, divergence of velocity, sources and sinks, and changes in saturated thickness using the new particle locations.
- Average the effects of b and d, and implement this average effect.

C. COMPUTER PROGRAM

The computer program is written in FORTRAN IV. A listing of the original code as written by USGS is found in the user's manual. This code has been modified slightly for implementation on the CYBER system. An overall flow-chart has been attached (Figure 5) and a list of the subroutines is shown in Table 1.

Several special provisions have been built into the program for particle accounting and movement. Particles are generated at sources with a line source character at aquifer boundaries and a divergent, point-source character in the aquifer interior. A special velocity interpolation is used near point sources and sinks. Particles can leave the aquifer only at specified sinks. If a particle's velocity carries it across an impermeable distribution is automatically redistributed and smoothed if it becomes uneven beyond a built-in criterion. The solute distribution has no such restriction.

The source program includes coding for a variety of boundary conditions. In Table 2, boundary and initial conditions of USGS-2D are listed. Most of the boundary conditions simulate continuous flow, but initial flow slug sources can also be simulated. Wells are treated as point sources or sinks, but the other boundary conditions are treated as distributed flow. Both head-independent and leaky artesian (head-dependent) sources and sinks are included. The latter can be limited-flow (leakance) cells or unlimited-flow (constant head) cells. Solute sources/sinks and concentration boundary conditions are included, though both must be tied to groundwater sources/sinks.

Table 2 also lists the boundary and initial condition options of the Random Walk and SUTRA programs. Discussions of those programs will refer back to Table 2. This table facilitates comparisons of the models.

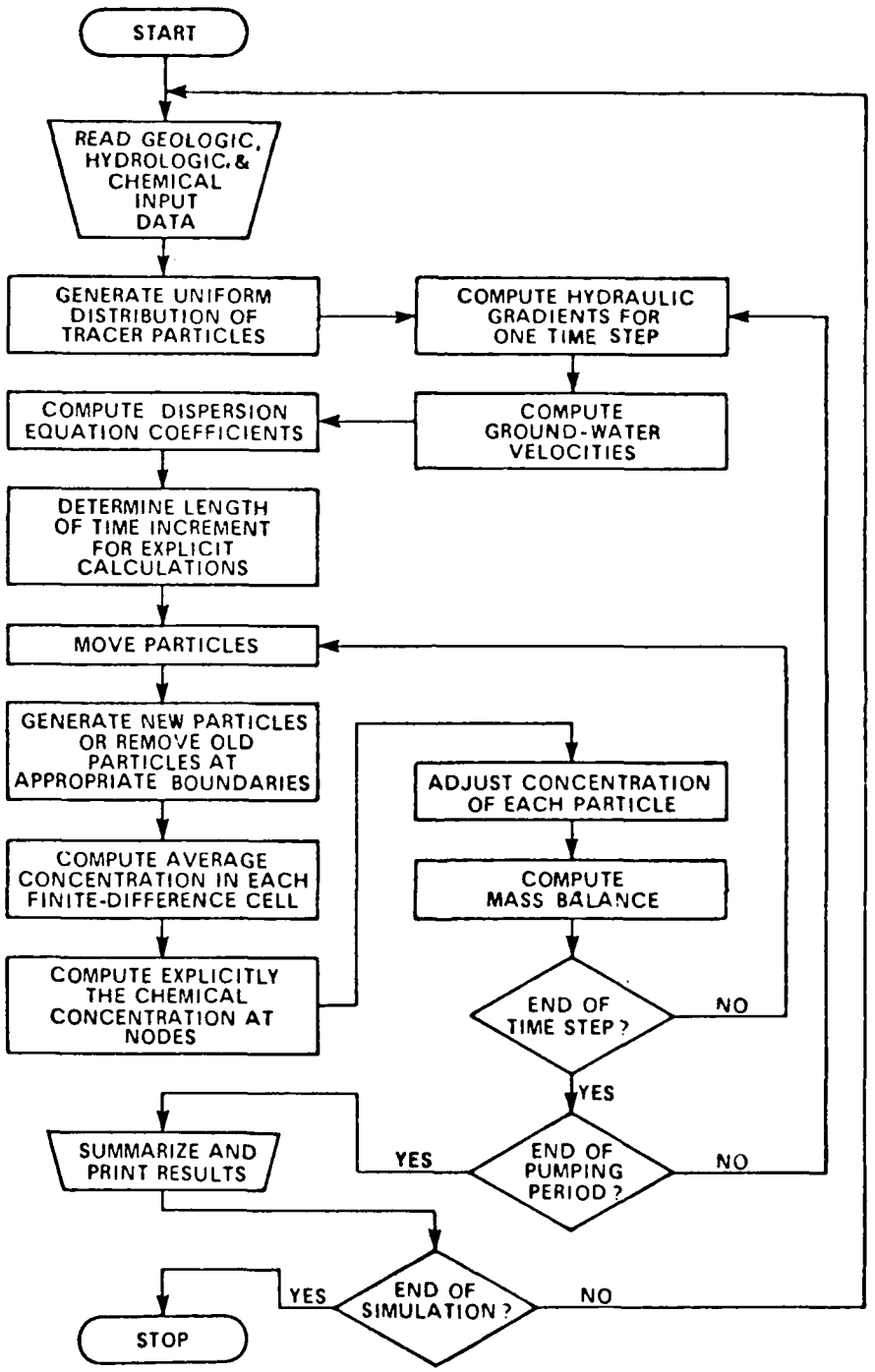


Figure 5. Simplified Flow Chart of the USGS Two-Dimensional Program (Reference 3).

TABLE 1. LIST OF SUBROUTINES FOR USGS-2D PROGRAM (REFERENCE 3).

Name	Purpose
MAIN	Control execution.
PARLOAD	Data input and initialization.
ITERAT	Compute head distribution.
GENPT	Generate or reposition particles.
VELO	Compute hydraulic gradients, velocities, dispersion equation coefficients, and time increment for stable solution to transport equation.
MOVE	Move particles.
CNCON	Compute change in chemical concentrations and compute mass balance for transport model.
OUTPT	Print head distribution and compute mass balance for flow model.
CHMOT	Print concentrations, chemical mass balance, and observation well data.

TABLE 2. BOUNDARY AND INITIAL CONDITIONS AND MODEL PARAMETERS FOR THE THREE GROUNDWATER MODELING PROGRAMS.[1]

PARAMETER	MODEL		
	USGS-2D	RANDOM WALK	SUTRA(2,3)
TIME DISCRETIZATION Number of Pumping Periods	NPMP	NRT	ITMAX
Durations Permitted	Uniform or nonuniform PINT(4) [years]	Uniform only [days] DELTA	Uniform or cyclic [seconds] (5)
Number of Time Steps Per Pumping Period: (for Head Calculations)	NTIM	NSP (6)	(7)
(for Solute Transport Calculations)	(see CELDIS)	(see DXMAX,DYMAX)	(7)
Length of Initial Time Step	TINIT [sec] (USS only)	Not an input parameter	DELT [sec]
Multiplier for Subsequent Steps	TIMX (USS only) [seconds]	Not an input parameter	DTMULT [seconds]
Maximum Length of a Time Step	N/A	Not an input parameter	TMAX [seconds]
Number of Time Steps in:			
Head Solution Cycle	N/A	NSP	NPCYC
Solute Solution Cycle	N/A	N/A	NUCYC
SPATIAL DISCRETIZATION: Number of Rows of Cells/Elements	NY	NR	N/A (8)
Number of Columns of Cells/Elements	NX	NC	N/A (8, 9)
Matrix Bandwidth	N/A	N/A	NBI (10)

TABLE 2. BOUNDARY AND INITIAL CONDITIONS AND MODEL PARAMETERS FOR THE THREE GROUNDWATER MODELING PROGRAMS (CONTINUED).

PARAMETER	MODEL		
	USGS-2D	RANDOM WALK	SUTRA(2)
Size of Elements: Length: Width:	YDEL XDEL [ft]	DELY DELX [ft]	Y(N)(11) X(N)(11) [m]
Theoretical Recommended Limits: (12)	XDEL, YDEL ≤ 4*BETA uniform cell size	DELX, DELY ≤ 4*DISPL variable cell size(13) (14)	Element length (or width) ≤ 4*DISPL. Size, like shape, can be variable (15)
Node/Cell Relationship	Nodes centered in cells	Nodes located at cell corners	Nodes located at element corners
Cell Thickness	N/A Directly enter saturated thickness--not aquifer thickness	((CH(i,j) - BOTT(i,j))	Aquifer thickness specified at nodes. In between nodes, thickness is interpolated by basis functions
Elevations:	Enter only THCK(i,j) Cells treated as if centered vertically about a horizontal plane.	Enter these elevations: CH(i,j) = top of aquifer BOTT(i,j) = bottom of aquifer	Cell thicknesses are specified directly, instead of elevations. Elements are vertically centered about a plane of symmetry. (16)
Sloped Aquifers:	Nothing in algorithm to handle slopes	(17)	GRAVX, GRAVY specify the effects of gravity on an inclined plane. (18)
Weighting Functions:	N/A	N/A	UP = 0 : Galerkin weighting (19) UP = 1 : Upstream asymmetric weighting (19)

TABLE 2. BOUNDARY AND INITIAL CONDITIONS AND MODEL PARAMETERS FOR THE THREE GROUNDWATER MODELING PROGRAMS (CONTINUED).

PARAMETER	MODEL		
	USGS-2D	RANDOM WALK	SUTRA(2)
Provisions for Wells: Are they handled differently from diffuse sources?	YES REC(i,j) for well rates YES RECH(i,j) for diffuse source rates (20)	YES P(i,k,t)for well rates YES and NO (21)	Wells may be included as boundary conditions, but SUTRA treats them as diffuse sources.
Particle velocity reinterpolated after moving a distance of: (x) (y)	CELDIS*XDEL CELDIS*YDEL (Built into automatic stability maintenance coding)	DXMAX*DELX DYMAX*YDEL (Currently, DXMAX and DYMAX are not input parameters.They are specified in the source code.	N/A (No moving particles are used.)
AQUIFER MATRIX PROPERTIES Hydraulic Conductivity or (Permeability) X Y (Hydraulic conductivity is also a function of fluid properties)	T(i,j)/THCK(i,j)[ft/sec] T(i,j) * ANFCTR [ft/sec] THCK(i,j)	PERM2(i,j) (xx) PERM1(i,j) (yy) [gal/day-ft^2]	(PMAX(L))along max perm. axis (PMIN(L))along min perm. axis (22) ANGLEX(L) angle between axes
Saturated Thickness	THCK(i,j) [ft]	thick(i,j) = MIN1((CE(i,j) - BOTT(i,j)),(H(i,j) - (BOTT(i,j))).Recalculated each iteration from default or array data. (23) [ft]	MIN1((H(N)-THCK(N)/2), THCK(N))
Can saturated thickness values be used to calculate transmissivity change with time?	NO (24)	YES (25)	YES

TABLE 2. BOUNDARY AND INITIAL CONDITIONS AND MODEL PARAMETERS FOR THE THREE GROUNDWATER MODELING PROGRAMS (CONTINUED).

PARAMETER	MODEL		
	USGS-2D	RANDOM WALK	SUTRA(2)
Transmissivity: X : Y :	T(i,j) T(i,j) * ANFCTR [ft^2/sec]	PERM(i,j,2) * thick(i,j) PERM(i,j,1) * thick(i,j) [gal/day-ft]	(26)
Anisotropy:	ANFCTR = $T_y(i,j)/T_x(i,j)$ (uniform over aquifer)	(y) T(i,j,1) = PERM(i,j,1) * thick(i,j) (x) T(i,j,2) = PERM(i,j,2) * thick(i,j)	Have axes of min and max permeability. Adjust permeability for flow direction.
Dispersivity: Longitudinal:	BETA [ft]	DISPL [ft]	DISPL(L) [m]
Transverse:	BETA * DLTRAT [ft]	DISPT [ft]	DISPT(L) [m]
Diffusivity: (Molecular)	N/A (normally included in dispersivity)	N/A (normally included in dispersivity)	SIGMAW [m^2/sec] (27)
Storativity: Artesian: Water Table:	S: one value for all cells, whether Artesian or Water Table conditions [unitless]	S1(i,j) [gal] (28) S2(i,j) [gal/ft]	No sto. vity input parameter
Aquifer Porosity: Volumetric: Effective:	POROS N/A	S2(I,J) groundwater flow APOR solute transport (29) EPOR (solute)	POR(N) N/A

TABLE 2. BOUNDARY AND INITIAL CONDITIONS AND MODEL PARAMETERS FOR THE THREE GROUNDWATER MODELING PROGRAMS (CONTINUED).

PARAMETER	MODEL		
	USGS-2D	RANDOM WALK	SUTRA(2)
Unsaturated Flow Parameters (30):	N/A	N/A	(30)
FLUID PROPERTIES: Density at reference composition	Assumed = 1.00 @ all solute concentrations [g/ml]	Assumed = 1.00 @ all solute concentrations [g/ml]	RHOWØ = reference density (31) URHOWØ = reference concentration DRWDU = density change w.r.t.comp.(31)
SOURCE TERMS: Groundwater flow rate head-independent diffuse source	RECH(i,j) [ft/sec]	Q(i,j) [gal/day]	QINC(t) (can change with time period) [kg/sec]
Groundwater Source Concentration	CNRECH(i,j) [ppm] FCTR2; Data Set #7	CONSOR(i,j) [ppm]	UINC(t) can change with time period [kg_s/kg_w]
Groundwater Leakance Coefficient (head-dependent sources)	FCTR1; Data Set # 7 [1/sec]	R(i,j) [gal/day/ft]	No leaky artesian conditions
WATER TABLE VALUES: Initial Conditions:	Data Set #8 WT(i,j) all cells [ft]	H(i,j) [ft]	PVEC (II) (m) (Unit 55)
Boundary Condition:	Data Set #8 WT(i,j) (leaky artesian cells only) [ft]	RH(i,j) (has effect only where R(i,j) > 0) [ft]	PBC(N,1) [m]

TABLE 2. BOUNDARY AND INITIAL CONDITIONS AND MODEL PARAMETERS FOR THE THREE GROUNDWATER MODELING PROGRAMS (CONTINUED).

PARAMETER	MODEL		
	USGS-2D	RANDOM WALK	SUTRA(2)
Closeness of pressure fit to specified pressure boundary conditions	N/A	N/A	GNUO a multiplicative factor to control closeness of fit
CONCENTRATION VALUES: Initial Condition:	Data Set #9; CONC(i,j) [ppm]	(32)	UVEC(NN) [mass fraction] (Entered in Unit 55)
Boundary Condition:	N/A	N/A	UINC(N,t) the solute concentration of the water that maintains the pressure or concentration boundary condition [mass fraction]
CONVERGENCE TOLERANCE: Groundwater Flow:	TOL single greatest change of any cell [ft]	ERROR the program sums the changes in head of all the cells during each iteration.SUM(n) ≤ ERROR [ft]	RPMAX [ft]
Solute Transport:	N/A a given set of input parameters always gives exactly the same results	N/A (33)	RUMAX [mass fraction]
ADSORPTION: Adsorption partition factor (concentration ratio of adsorbed to dissolved concentrations)	original program N/A	KD1 [lb/gal]	See adsorption models

TABLE 2. BOUNDARY AND INITIAL CONDITIONS AND MODEL PARAMETERS FOR THE THREE GROUNDWATER MODELING PROGRAMS (CONCLUDED).

PARAMETER	MODEL		
	USGS-2D	RANDOM WALK	SUTRA(2)
Retardation factor	N/A	RD1 = 1. + K_d*RHO/EPOR	N/A
Adsorption Model:	original program: none in revised DOE program: linear, Freundlich, & Langmuir adsorption models	linear only (in retardation factor model)	ADSMOD (34) ID of adsorption model (linear, Freundlich Langmuir) CHI1, CHI2: adsorption model parameters
Density of Solid Matrix Grains (Affecting only retardation/ adsorption calculations)	N/A	RHO	RHOS
REACTION TERMS: (Chemical, Biochemical and Nuclear combined)	N/A (not in basic version)	N/A (user will empirically try to use RD1, instead)	PRODFO [kg_s/kg_w-sec] PRODF1 [1/sec] PRODSO [kg_s/kg_G-sec] PRODS1 [1/sec] (35)

PARAM implies a parameter constant over time and over the aquifer.
PARAM(t) implies a parameter constant over the aquifer, varying over time.
PARAM(i,j,) implies a parameter constant over time, varying over the aquifer.
PARAM (i,j,t) implies a parameter varying over time and the aquifer.
PARAM(N) implies a SUTRA parameter discretized by node. (may be handled internally by node or (SUTRA) cell).
PARAM(L) implies a SUTRA parameter discretized by element.

(1) More details and user instructions are given in appendices and in user manuals.

(2) Will use footnotes to differentiate between SUTRA `82 and `84 where necessary.

(3) Units in SUTRA can be metric (mks) or English. User must inter-convert carefully.

(4) PINT is read in and updated each time period.

(5) Pumping periods are the same as time steps in SUTRA.

(6) May speed up convergence in unsteady state cases.

(7) Time steps are program-wide. Pumping rates can be constant, can change every time period, or can change however the user specifies in subroutine BCTIME.

(8) The finite element mesh will still have columns and rows. However, because the elements are permitted to have arbitrary quadrilateral shapes, the rows and columns need not be straight, perpendicular, or of uniform length. Because of that, SUTRA elements and nodes are each indexed sequentially in one dimension, rather than by row and column number, and NC and NR are no longer included as input parameters.

(9) An "element" in SUTRA is similar to a cell in Random Walk, with a node at each corner. A "cell" in SUTRA is centered on a node, and extends half way to the four closest nodes, like a cell in USGS-2D

(10) Full matrix bandwidth is a good indicator of the core storage needed. To calculate bandwidth:
- for each element calculate the difference between the highest and lowest node index number
- let DD = the greatest such difference in any element in the mesh
- NBI = 2 * DD + 1

(11) Node positions are specified directly, and the program calculates the size of the elements based on the node positions and the connectivity data (specified later in the input file)

(12) Computer system core limitations may require a smaller number of larger elements.

(13) Cell length should be uniform within each row, and cell width should be uniform within each column.

(14) Cell length (width) should not change by a factor of more than 2.0 between adjacent rows (columns).

(15) Plume width should be at least ten times element width. There should be at least five elements across a moving concentration front.

(16) The plane of symmetry is flat (no curvature, bumps, folds, etc.) but may be inclined from the horizontal.

(17) The program has the geometric input parameters to handle a sloping aquifer, but not the coding to calculate the effects of gravity on water flow in a sloping aquifer.

(18) The plane of symmetry is most commonly horizontal, but may be sloped, a well. The program can handle a sloped aquifer The tilt from horizontal is handled by the orientation vector components GRAVX, GRAVY. Gravitational effects of the tilt on flow will automatically be included in the calculations.

(19) See SUTRA user's manual. Default (symmetric) is Galerkin weighting. Asymmetric option is Galerkin-Petrov weighting.

(20) The values stored in REC(i,j) are updated each time period by Data Set 10C.

(21) Q(i,j) are diffuse sources, stored nodewise. Each pumping period, (P(i,j,t) + Q(i,j)) is read into the Q(i,j) array, with (P(i,j,t) + Q(i,j)) replacing Q(i,j) only at nodes with pumps. From there on, point and diffuse sources are treated the same.

(22) The permeability value used is adjusted for the direction of flow relative to the minimum and maximum permeabilities and their directional axes.

(23) Default data is uniform in space and time. Array data can vary freely by cell: Only H(i,j) can vary with time.

(24) Water table levels can change, but will not affect the saturated thickness values used to calculate cellwise transmissivity.

(25) After each iteration, a FORTRAN minimum function, MIN1((CH(i,j) - BOTT(i,j)), (H(i,j) - BOTT(i,j))) is used to calculate the saturated thickness of each cell.

(26) Not a SUTRA input parameter. Uses the product of permeability and saturated thickness.

(27) Molecular diffusivity is one component of overall dispersivity. In most groundwater cases, molecular diffusivity is only a negligible factor. The Konikow and Random Walk models do not even bother with diffusivity. SUTRA includes a diffusivity input parameter, which can usually be set to zero.

(28) Storativity is related to porosity.
- Under Artesian conditions, storativity is due to the change in porosity with changing head
- Under water table conditions, storativity =
  - porosity, when water level rises, or
  - volume percent free drainage, when water level falls

(29) SF2 is used in the head solution portion of the program; APOR & EPOR are used in the solute transport portion.

(30) The USGS-2D and Random Walk programs can handle only saturated flow. SUTRA was written primarily for saturated flow, but can handle some unsaturated flow problems, too. The unsaturated flow parameters are explained in the manual, but are mentioned only in passing in this table because no unsaturated flow modeling work was performed in this project.

(31) Reference solute concentration is usually zero. Reference density of water is usually 1000 kg/m^3.

(32) Concentration arrays are always initialized with 0 concentration. Options for non-zero concentrations include:
- revising one of the initialization subroutines to produce the required initial concentration distribution
- using the first time period to establish the initial concentration distribution (could use a subroutine such as GENP(PL) only once, during the first time period, to establish nonzero initial concentration conditions)
- using transformed concentration variables, where the transformed concentration variable = 0 when the concentration is at its initial value.

(33) Due to the random dispersional movements of the particles, a given input data file will give slightly different results each time it is run.

(34) See SUTRA manual for explanations of models. CHI1 and CHI2 will be defined according to the model used.

(35) Chemical reaction kinetic constants:
- PRODF0 = zeroth order production/consumption in aqueous phase
- PRODS0 = zeroth order production/consumption in adsorbed phase
- PRODF1 = first order production/consumption in aqueous phase
- PRODS1 = first order production/consumption in adsorbed phase

SECTION III

THE ILLINOIS RANDOM WALK MODEL

The "Random Walk" (RW) model is a finite difference model for groundwater flow coupled to a moving particle model for solute transport (References 5, 6). The particle model uses a random walk algorithm to represent solute dispersion. For steady-state groundwater flow, the flow and solute models can be solved separately. The model features an areal, two-dimensional rectangular grid with nodes located at the corners of the cells. A sample grid and cell are shown in Figure 6 and 7, respectively. The solute can either be conservative or retarded by adsorption.

The grid is rectangular, but column and row widths may vary. The restrictions are:

- in each row (column), the cells can have only one length (width).
- in any two adjacent rows (columns), the cell length (width) should not vary by more than a 2:1 ratio.

The program is entitled "A Random Walk Solute Transport Model for Selected Groundwater Quality Evaluations." It was written by Prickett, Naymik, and Lonnquist of the Illinois State Water Survey (Reference 6). This 1981 version is available at low cost for use on mainframe and minicomputers. Dr. Prickett is now an independent consultant, and has written later versions of his program for use on a personal computer.

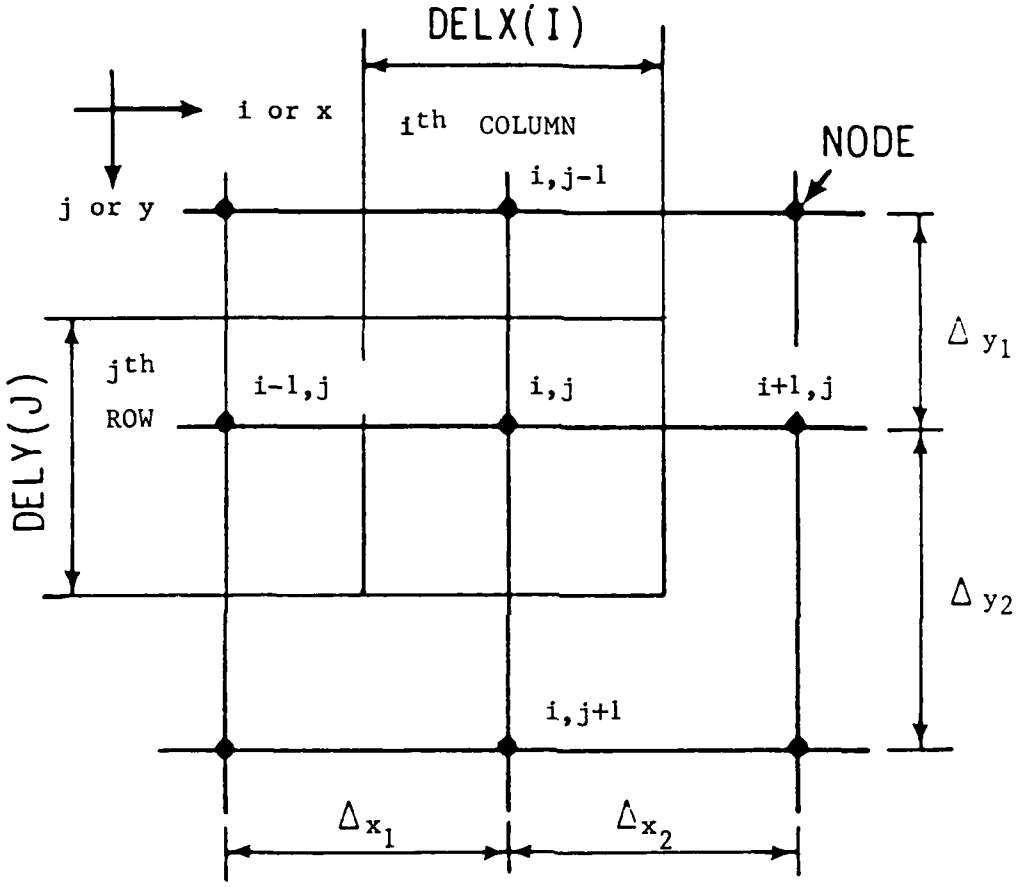
A. FLOW ROUTINE

The groundwater flow routine, an update of the 1971 model of Prickett and Lonnquist (Reference 5), is normally used for areal simulations. It uses a Modified Iterative Alternating Direction Implicit (MIADI) algorithm similar to that in USGS-2D (Reference 3). Groundwater flow is assumed to obey Darcy's Law (Equation (1)). The acceptable classes of boundary conditions are similar to USGS-2D: constant head, specified (constant) leakance coefficient, specified diffuse flow, and extraction/recharge wells. These boundary conditions are discussed in Table 2, where they are compared to boundary conditions used in USGS-2D and SUTRA. These boundary conditions are also illustrated in Figure 8.

1. Governing Equation

The differential equation for groundwater flow is (Reference 6):

$$\underbrace{\frac{\partial}{\partial x}\left[K_x\, b\, \frac{\partial h}{\partial x}\right]}_{\substack{\text{(pore flow,}\\ \text{x-direction)}}} + \underbrace{\frac{\partial}{\partial y}\left[K_y\, b\, \frac{\partial h}{\partial y}\right]}_{\substack{\text{(pore flow,}\\ \text{y-direction)}}} = \underbrace{S\,\frac{\partial h}{\partial t}}_{\text{(storage)}} + \underbrace{Q}_{\text{(source)}} \qquad (9)$$



$$DELX(I) = .5\,(\Delta x_1 + \Delta x_2)$$

$$DELY(J) = .5\,(\Delta y_1 + \Delta y_2)$$

Figure 6. Finite Difference Grid (Reference 6).

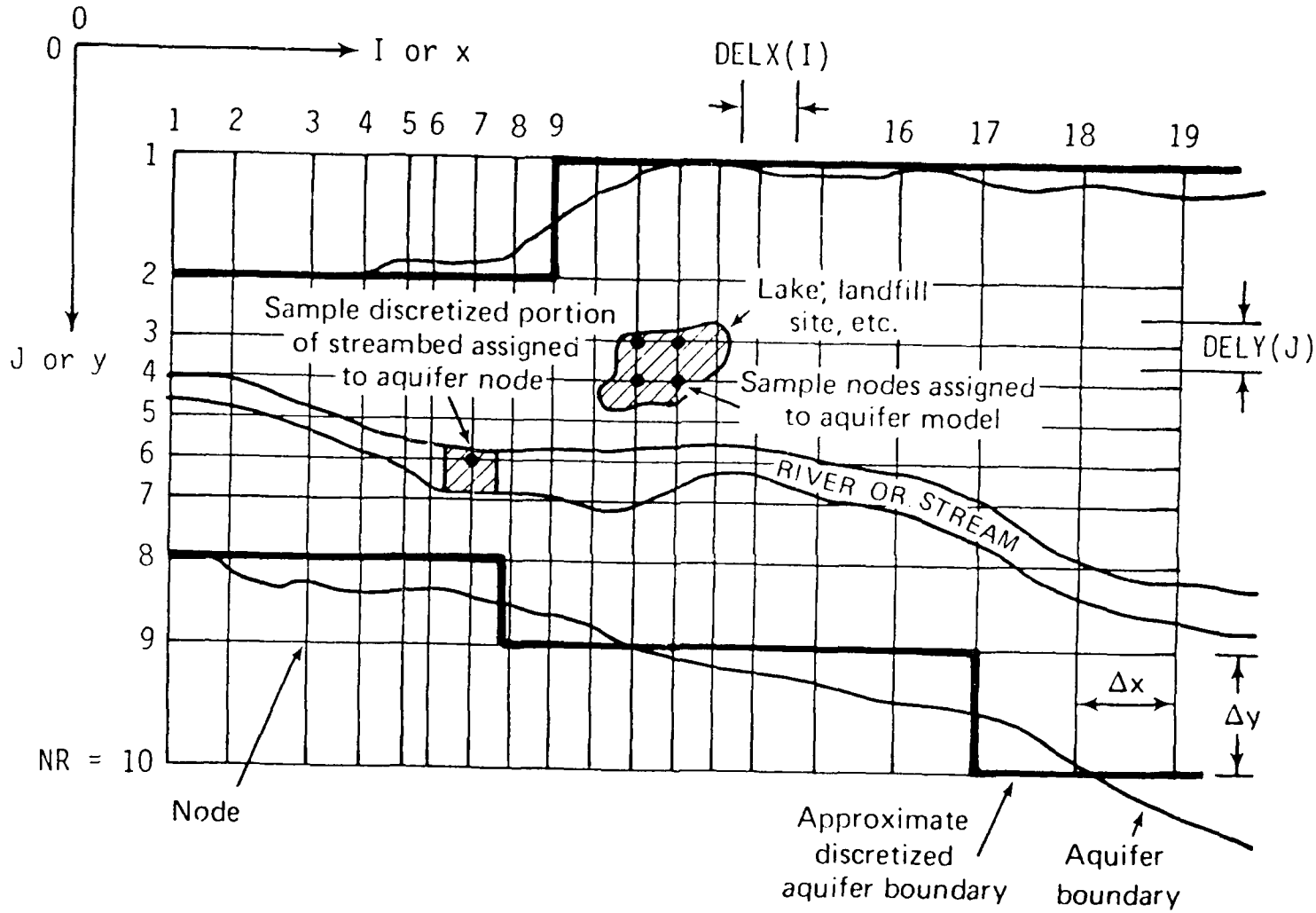


Figure 7. A Sample Aquifer System (Reference 6).

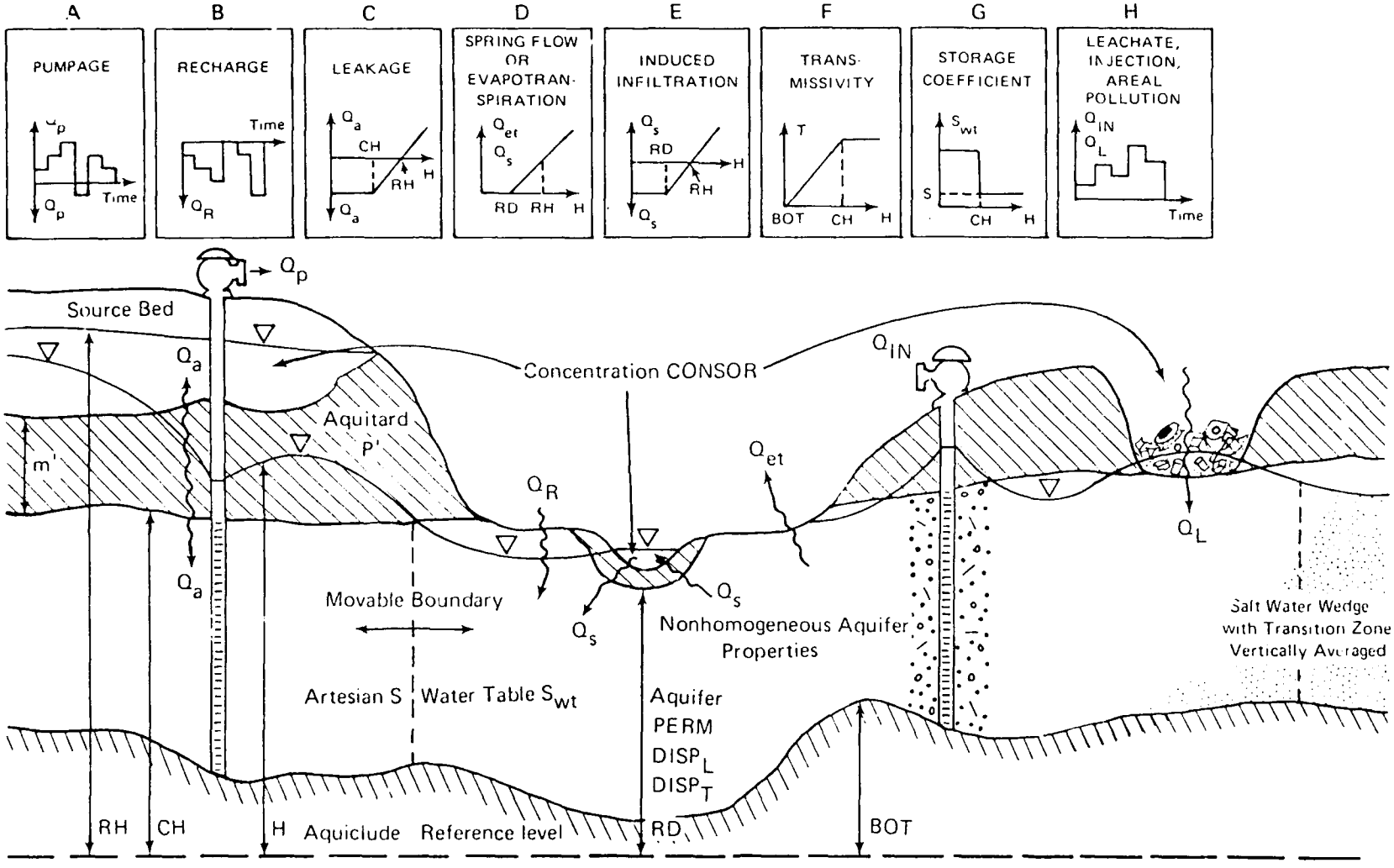


Figure 8. Generalized Aquifer Cross Section Showing Simulation Program Parameters and Boundary Conditions (Reference 6).

where:

K_x = hydraulic conductivity, x-direction

K_y = hydraulic conductivity, y-direction

b = aquifer thickness at a node

h = hydraulic head

S = storativity

Q = source/sink function = Q(x,y).

2. Parameters for the Numerical Solution of Equation (9)

The program's various input parameters are assumed constant over the space dimensions and time. For example, the two spatial discretization parameters, the number of columns (NC) and the number of rows (NR) are constant over time and space, as are the following two simulation parameters: the MIADI time increment (DELTA) and the MIADI convergence tolerance (ERROR).

B. SOLUTE ROUTINE

1. Background

Solute transport in the Random Walk Program is governed by the same basic differential equation used in the USGS-2D program (Equation (4)). This equation was derived for a stationary coordinate system, as used in USGS-2D and in the RW groundwater flow routine. Solute transport can also be analyzed using a coordinate system moving with the average velocity of the groundwater. Because solute transport analysis in the RW program is based on such a moving frame of reference, the RW solute transport algorithm differs, correspondingly, from the USGS-2D algorithm.

While the RW program's groundwater flow routine keeps track of groundwater fluxes into and out of finite difference cells, the solute transfer routine tracks moving solute particles. Each particle represents PM pounds of pure solute, and its motion is governed by an advective velocity field, a random dispersion, and possible adsorption effects. The velocity field is based on the head distribution from the MIADI routine, Darcy's Law, and a velocity interpolation algorithm. Dispersion (modeled as random particle motion), adsorption (modeled as a retardation or slowing of particle motion), and solute sources and sinks are discussed in the following subsection.

2. Numerical Solution

The solute transport routine is both similar to and different from the USGS-2D model (References 3, 6). Both use particle models and both simulate advective transport using the groundwater head distribution from the ADIP/MIADI routine. One difference is the velocity interpolation

scheme. Random Walk (RW) interpolates with a set of three linear Chapeau functions, which use the velocities at the eight closest nodes, except at the edges and corners of the aquifer's domain of computation.

Random Walk adds particles at sources, and removes them at sinks. These sources and sinks differ in their details from those in USGS-2D. In the RW program, various subroutines can introduce solute in specified patterns (e.g., rectangles, lines, circles, and points) or as solute dissolved in source streams. Solute dissolved in source streams enters at the concentration specified by cell in array CONSOR(I,J), and exits at the prevailing cell concentrations.

The maximum number of particles allowed in the aquifer, MAXP, and the particle mass, PM, are interrelated. When the total number of particles present in the aquifer is less than MAXP, PM remains constant and the number of particles increases. When MAXP particles are present, the number of particles cannot grow and PM increases instead.

Dispersion is resolved into longitudinal and transverse components. Each component is proportional to $[(DISP_i)|V|]^{-1/2}$, and to a random number, ANORM. ANORM, which varies from +6 to -6, represents standard deviations of dispersional motion, and is generated in function ANORM. There, 12 random numbers, each ranging from -1 to +1, are generated and summed, and 6.0 is subtracted from this sum.

Longitudinal and transverse dispersivities are vectorially additive. Each is calculated in the longitudinal and transverse directions and resolved into X and Y components. The X and Y components of both vectors are added to yield dispersive motion. Molecular diffusion is generally quite small by comparison, and is assumed to be included in the dispersion coefficients. Particle movements for dispersion are added to those for convection.

Retardation is an indirect way to express the effects of adsorption. Due to adsorption, a solute will migrate more slowly than an otherwise equivalent conservative solute. The retardation factor is defined as (Reference 6):

$$RD1 = V_s/V = 1.0 + (KD)(RHO)(EPOR)^{-1} \qquad (10)$$

where:

RD1 = retardation factor at some location,

V_s = velocity of a concentration contour line,

V = groundwater velocity,

KD = adsorption partition coefficient = C_s/C,

C_s = concentration of solute in the adsorbed phase,

C = concentration of solute in the aqueous phase,

RHO = bulk mass density of the solid matrix,

EPOR = effective porosity of the matrix.

C. COMPUTER PROGRAM

The computer program, written in FORTRAN IV, contains approximately 1900 lines (including blank lines inserted for readability). The input parameters are read in during the main routine, TRANS (Figure 9). A list of subroutines is shown in Table 3. Flowcharts for the individual routines can be found in the user's manual (Reference 6). The groundwater head calculations (MIADI) are performed in Subroutine HSOLVE. Solute transport calculations require several different subroutines, which must be sequenced by the user.

While there is no built-in default sequence, the following is suggested:

- Initialization Subroutine, INIT, called from TRANS, before any particle movements.
- A DO Loop within TRANS to control iterative steps, consisting of:
  1. Subroutine CLEAR to initialize particle map arrays.
  2. Subroutine ADVAN to move the particles.
  3. Subroutine MAP and/or CONMAP to print plume maps of solute particles and/or solute concentrations.
  4. Subroutines SUMMRY and/or SNKCON, to print out particles captured by sinks and/or sink concentrations.
  5. Source generation subroutines.

All solute movement is calculated by particle movements. During each time period, Subroutine ADVAN steps through the particle arrays. For each particle, ADVAN calls Subroutine MOVE to execute the particle's convective and dispersive motion. Particle velocity is calculated by interpolation based on particle position at the beginning of the time period. The particle may move until the period is up, or movement may be interrupted once the particle has moved a distance greater than DXMAX or DYMAX (specified fractions of cell length or width). When movement is interrupted, velocity is recalculated and the move is continued. The particle is then moved by the random walk algorithm to simulate dispersion. If the preceding movements carry a particle beyond a boundary of the aquifer, the particle is immediately returned to that boundary.

MOVE also determines whether a particle is captured by a sink node. It locates the node closest to the particle and determines if that node is a sink node. If so, the subroutine determines if the particle has come within 1/2 cell of the sink, in either the X or Y direction. If so, the particle is removed from the aquifer and placed in that sink. Thus, the default "capture area" of a sink node is a full cell, centered on that node. If

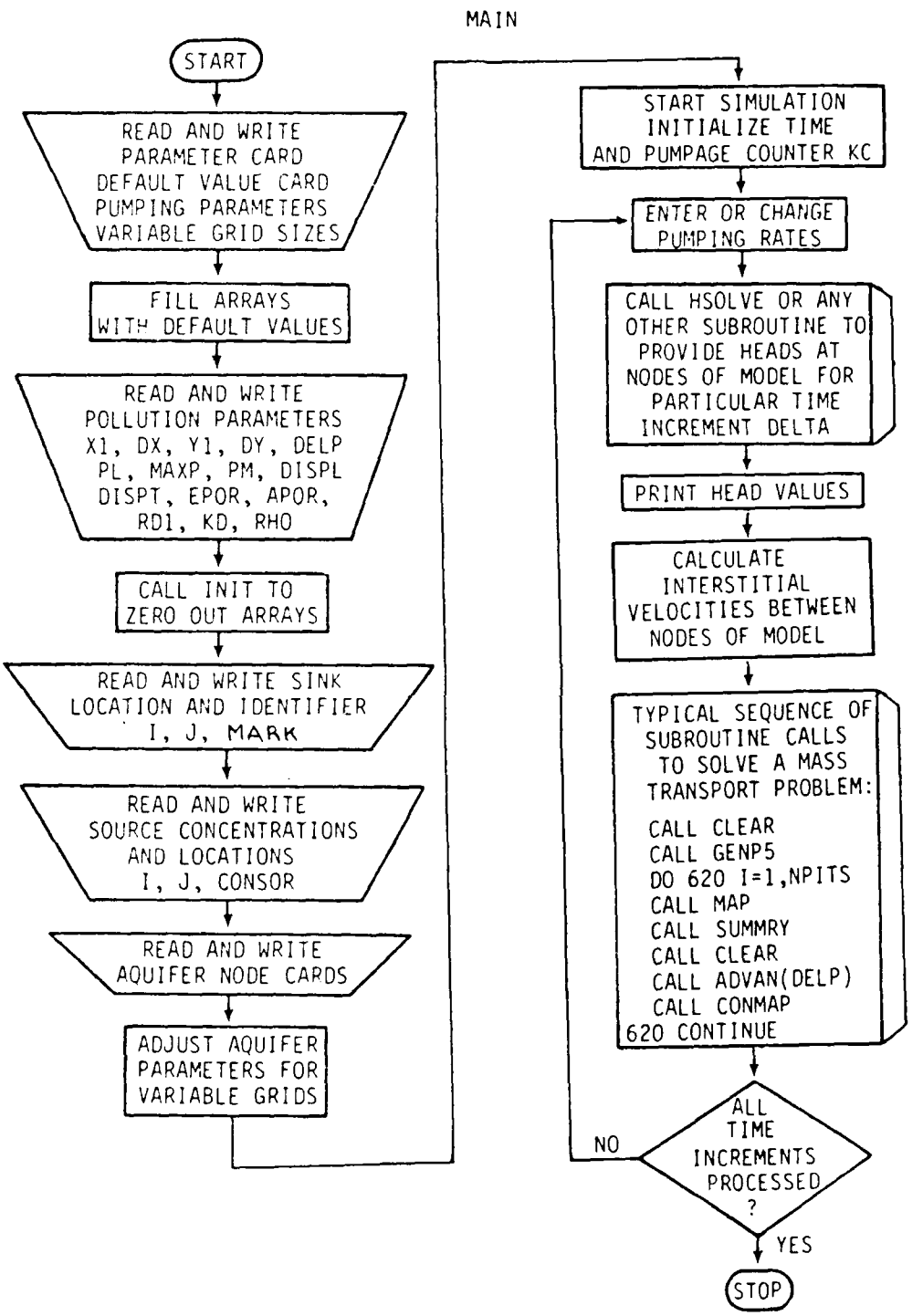


Figure 9. Flow Chart for Illinois Random Walk Program, Main Routine (Reference 6).

TABLE 3. BRIEF DESCRIPTIONS OF SUBROUTINES AND FUNCTIONS IN THE RANDOM WALK PROGRAM (REFERENCE 6).

ADD(XX,YY):	add single particle at coordinates (XX,YY)
ADVAN(DELP):	advances all particles DELP days
ANORM(0):	produces a single number from a normal distribution of mean 0, σ=1, range +6 to -6
CLEAR:	clears arrays NPART and TABLE
CONMAP:	prints concentrations at all nodes of model
GENP(PL):	produces PL/PM particles randomly in a rectangle X1,Y1,DX,DY and randomly in time increment DELP
GENP2:	generates 29 particles along column 30 of model, 1 particle per node
GENP3:	generates 51 particles, all at coordinate XX = 1, YY = 2
GENP4:	generates 360 particles around an R = 0.7 circle with center at coordinates (15,15), randomly during DELP
GENP5:	generates 101 particles around an R = 0.7 circle with center at coordinates (15,15), at the onset of the call
HSOLVE:	ISWS Bulletin 55 (Prickett and Lonnquist, 1971), composite program
HSOLV2:	calculates linear heads per grid left to right
HSOLV4:	Thiem equation, radial flow from an injection well at coordinates (15,15)
INIT:	initializes or zeros out arrays TMAP, NP, ANC, ANR, SOR, CONSOR, and MARK
MAP:	prints number of particles residing in each zone for whole model
MOVE(XX,YY,DEL):	moves particles and tabulates in which zone particle resides and removes particles when captured by a sink
RDSOLV(EPOR,RHO,KD,RDI):	calculates retardation factor from input data
SNKCON:	for time DELP, prints concentration at sinks specified by MARK
SORGEN:	produces particles based on either head dependent flow rates or injection wells randomly in space in time during DELP
SOURCE:	produces particles when particle mass has sufficiently accumulated from any source
SUMMRY:	prints out number of particles captured by a sink during time DELP
V:	provides proper velocities to subroutine VELO
VELO(XX,YY,VX,VY):	calculates interpolated velocities for particle movement

necessary, the user could modify the program to empirically adjust the capture area.

The following solute transport parameters, found on the "Pollution Parameter Card" (Appendix E), are to be assumed uniform over both time and all cells: longitudinal dispersivity (DISPL), transverse dispersivity (DISPT), effective porosity (EPOR), volumetric porosity (APOR), retardation coefficient (RD1), adsorption partition coefficient (KD), and matrix bulk density (RHO).

The following input parameters, specified by cell, are treated as uniform over time: storativity under artesian conditions (S1(I,J)), storativity under water table conditions (S2(I,J)), fixed recharge/leakage rate Q(I,J), leakance coefficient R(I,J), pond/river surface elevation RH(I,J), pond/river bottom elevation RD(I,J), aquifer top elevation CH(I,J), aquifer bottom elevation BOT(I,J), and hydraulic conductivity PERM(I,J,1) (y) and PERM (I,J,2) (x). In addition, the sink sizes and locations, and the source locations and concentrations are treated as constant over time.

The program contains a variety of particle generation subroutines, several of which generate special particle patterns (Table 4).

TABLE 4. PARTICLE GENERATION SUBROUTINES IN RANDOM WALK PROGRAM.

For Test Patterns:

- GENP2 generates 29 particles along column 30 of the grid, 1 particle per node.
- GENP3 generates 51 particles, all at coordinate (1,2).
- GENP4 generates 360 particles randomly during DELP around a circle of R = 0.7, centered at coordinates (15,15).
- GENP5 generates 101 particles at the beginning of DELP around a circle of R = 0.7, centered at coordinates (15,15).

For Real Simulation Sources:

- GENP generates (PL/PM) particles randomly within the rectangle [(X1,Y1),(X1+DX),Y1),(X1,Y1+DY),(X1+DX,Y1+DY)], randomly during DELP.
  - if DX = DY = 0, GENP simulates a point source.
  - if DX OR DY = 0, GENP simulates a line source.
- SOURCE generates particles within a groundwater source. Another particle is generated each time a specified mass of groundwater has been injected into the aquifer.
- SORGEN generates particles within a groundwater source, either a leakance source or an injection well. The number of particles generated during each time period is proportional to the source flow rate and concentration. However, within each time period, these particles are generated randomly within a specified space and time.

SECTION IV

THE SUTRA MODEL

A. INTRODUCTION

1. Purpose

SUTRA (Saturated-Unsaturated Transport) is a computer program which simulates fluid movement and transport of either energy or dissolved substances in a subsurface environment. The model uses a two-dimensional hybrid finite-element and integrated finite-difference method to approximate the governing equations which describe the two interdependent processes: flow of water plus solute, or flow of water plus thermal energy.

The program models groundwater flow produced by hydraulic gradients and various sources and sinks. It models the transport processes of advection, dispersion, adsorption, and chemical reaction (including biochemical reaction and/or radioactive decay). The boundary conditions can consist of specified heads, specified concentrations (or temperatures), specified groundwater sources (with or without solute), and specified solute sources (without groundwater). The boundary conditions may be constant, or may change with time. Initial conditions are also specified.

2. Model Applications

SUTRA can simulate both saturated and unsaturated flows. The program has all the I/O coding and algorithms needed to perform unsaturated flow simulations. However, because the program was designed primarily for saturated flow, unsaturated flow calculations are usually inefficient and often require fine spatial discretization and short time increments.

Groundwater flow may be steady- or unsteady-state. In unsteady-state flow problems, it may be necessary to solve both equations during each iteration. However, when the flow pattern changes slowly with time, the solution of the flow equation is only required every Nth iteration, where N is a specified integer. Unsteady-state problems generally require iterative calculations, though simpler once-through calculations may be used if the density, saturation, viscosity, and adsorption correlations are linear. In steady-state flow problems, the flow equation is solved only once.

SUTRA was structured for general applicability, numerical robustness, numerical accuracy, and clarity and modularity in coding. However, calculational speed and efficiency sometimes suffer as a result of this structure. The program has a general framework, but subroutines and coding for certain desirable options have not yet been implemented.

SUTRA was designed for two-dimensional simulations. Such simulations are usually areal simulations (Figure 10); however, vertical cross-sectional simulations can also be set up (Figure 11). Radial (cylindrical) flow can also be simulated (Figure 12). In each case, the gravity vector, g, shows the physical orientation of the mesh. Gravitational effects (on nonhorizontal flows) are automatically included in the calculations.

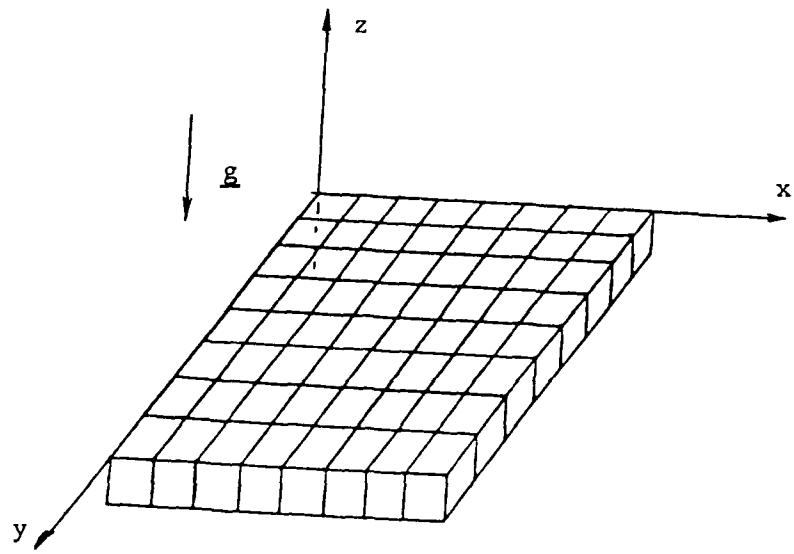


Figure 10. Two-Dimensional Rectangular Mesh.

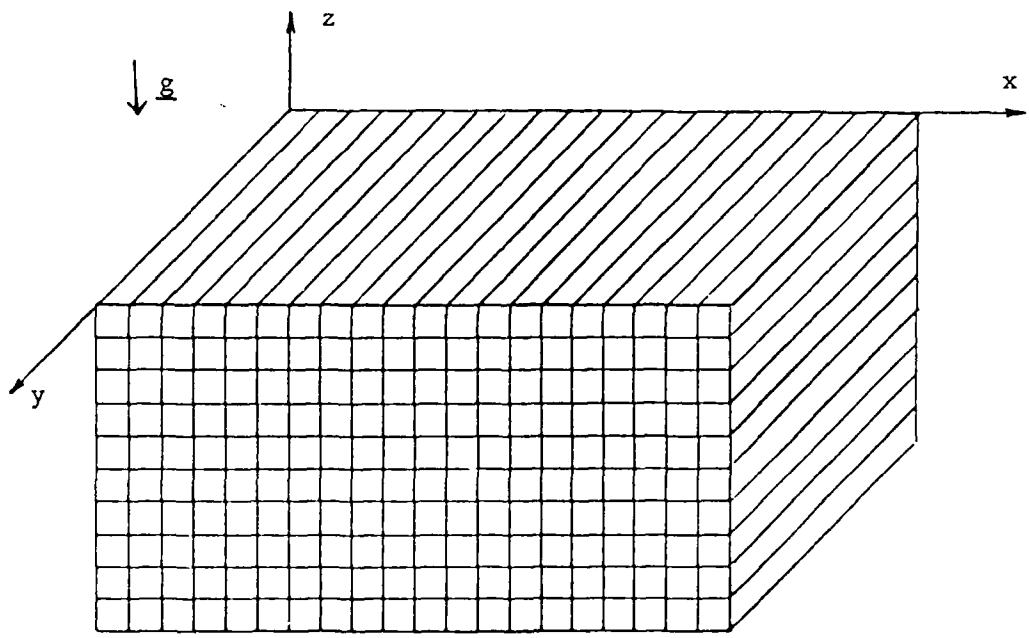


Figure 11. Two-Dimensional Vertical Cross-Sectional Rectangular Mesh.

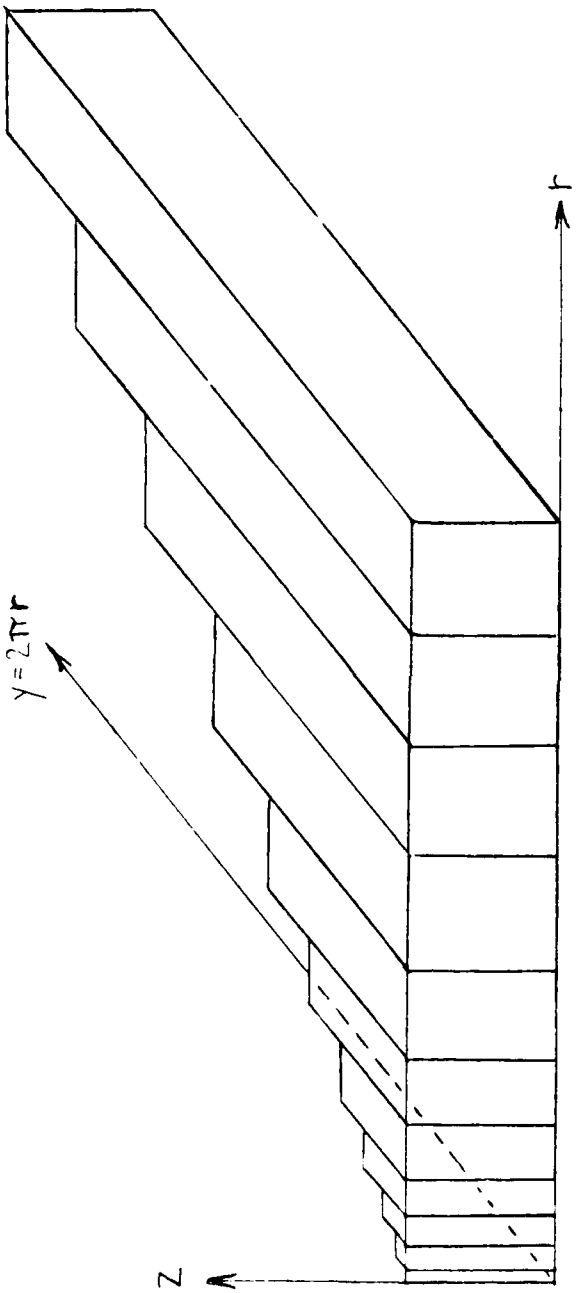


Figure 12. Two-Dimensional Cross-Section Radial Flow

Solute transport applications include analysis of aquifer test results, contaminant plume movement, aquifer restoration, and salt water intrusion. Energy transport applications include geothermal energy development, subsurface heat conduction, and natural hydrologic convection situations.

As in any modeling, the quality of the output depends on the quality of the input data. Complete, quantitative solutions require a properly discretized mesh, a complete set of input data, and a modeling program capable of properly representing the boundary conditions. When less input data is available, semiquantitative solutions can be used to guide the placement of test wells for additional data collection, and to test certain modeling assumptions.

B. GOVERNING EQUATIONS

1. Groundwater Flow Equations

a. Darcy's Law and Fluid Velocity

The tensor form of Darcy's Law for saturated conditions is given by:

$$\underline{v} = - (\underline{\underline{K}}/\varepsilon \cdot \underline{\nabla} h) \tag{11}$$

where:

$$h = \frac{p}{\rho |\underline{g}|} + \text{elevation.} \tag{12}$$

The parameters and variables in Equations (11) and (12) are defined as:

$\underline{v}$ = velocity vector,

$\underline{\underline{K}}$ = hydraulic conductivity tensor (m/sec),

$\underline{\nabla}$ = gradient operator,

ε = aquifer porosity,

ρ = density of groundwater,

h = hydraulic head, and

$\underline{g}$ = gravitational acceleration vector, given by:

$$\underline{g} = - |g| \cdot \underline{\nabla} (\text{elevation}). \tag{13}$$

Darcy's velocity for unsaturated conditions is given by:

$$\underline{q} = \varepsilon S_w \underline{v} \tag{14}$$

where S_w is the fractional saturation of the soil, or the volume of water per volume of voids, and satisfies $0 < S_w \leq 1$. The soil matrix is "bone dry" when $S_w = 0$, and at full saturation when $S_w = 1$.

If a volume of saturated matrix is allowed to drain freely, S_w will fall to S_{wres}, the residual saturation. Groundwater flow ceases at this point because the remaining water is tightly bound in place by surface tension in isolated favorable spots. At intermediate saturation values, saturation and vacuum pressures can be related by the Van Genuchten Equation, an empirical correlation (Reference 8):

$$\frac{dS_w}{dp} = \frac{a(n-1)\left[1 - S_{wres}\right]\left[a\,p_c\right]^{(n-1)}}{\left[1 + \left[ap_c\right]^n\right]^{\frac{2n-1}{n}}} \qquad (15)$$

where:

a, n = empirical constants,

$p_c = p_{ATM} - p$ = capillary pressure,

p_{ATM} = atmospheric pressure, and

p = fluid pressure in the soil matrix.

b. Hydraulic Conductivity and Permeability

While hydraulic conductivity, $\underline{\underline{K}}$, is a useful property and can be measured directly in the field, it is a property of both the aquifer matrix and the flowing fluid (i.e., it varies with viscosity and fluid density). Permeability (hydraulic conductivity at standard flow conditions) is a property of the aquifer matrix alone. Permeability is defined in tensor form as:

$$\underline{\underline{K}} = \underline{\underline{k}}\, k_r\, \gamma/\mu \qquad (16)$$

where:

$\underline{\underline{k}}$ = permeability (m^2),

k_r = relative permeability factor,

μ = fluid viscosity (kg/m-sec), and

γ = specific weight ($kg/m\text{-}sec^2$) = ρg.

In two dimensions, $\underline{\underline{k}}$ can be resolved in terms of (x,y)-coordinates or (x_p, x_m)-coordinates, where the latter system consists of axes along the directions of maximum k, ($k = |\underline{\underline{k}}|$), and minimum k (Figure 13). The user enters by element into SUTRA's input data file, the maximum and minimum permeability values, and the angle between the x-axis and the axis of the maximum permeability. SUTRA automatically calculates permeability in the flow direction. This is referred to as "rotation of the permeability tensor."

The relative permeability, k_r, can also be calculated from a Van Genuchten Equation:

$$k_r = \sqrt{S_w^*} \left[1 - \left(1 - S_w^{* \left[\frac{n}{n-1}\right]} \right)^{\left[\frac{n}{n-1}\right]} \right]^2 \qquad (17)$$

where S_w^* = dimensionless saturation given by:

$$S_w^* = \frac{S_w - S_{wres}}{1 - S_{wres}} . \qquad (18)$$

c. Fluid Density

Differences in fluid pressure (p) or head (h) are the primary driving forces for groundwater flow; however, differences in density can be a secondary driving force. Differences in density can be caused by differences in temperature or solute concentration.

In SUTRA, it is assumed that the fluid density as a function of temperature, $\rho(T)$, or as a function of concentration, $\rho(C)$, can be approximated by the linear terms of its Taylor expansion, namely:

$$\rho = \rho_o + \frac{d\rho}{dT} \left(T - T_o \right) , \qquad (19)$$

or:

$$\rho = \rho_o + \frac{d\rho}{dC} \left(C - C_o \right) \qquad (20)$$

where:

ρ_o = reference density, usually the density of pure water,

T = reference temperature,

C_o = reference solute concentration, usually zero for pure water,

C = solute concentration in kg of solute per kg groundwater.

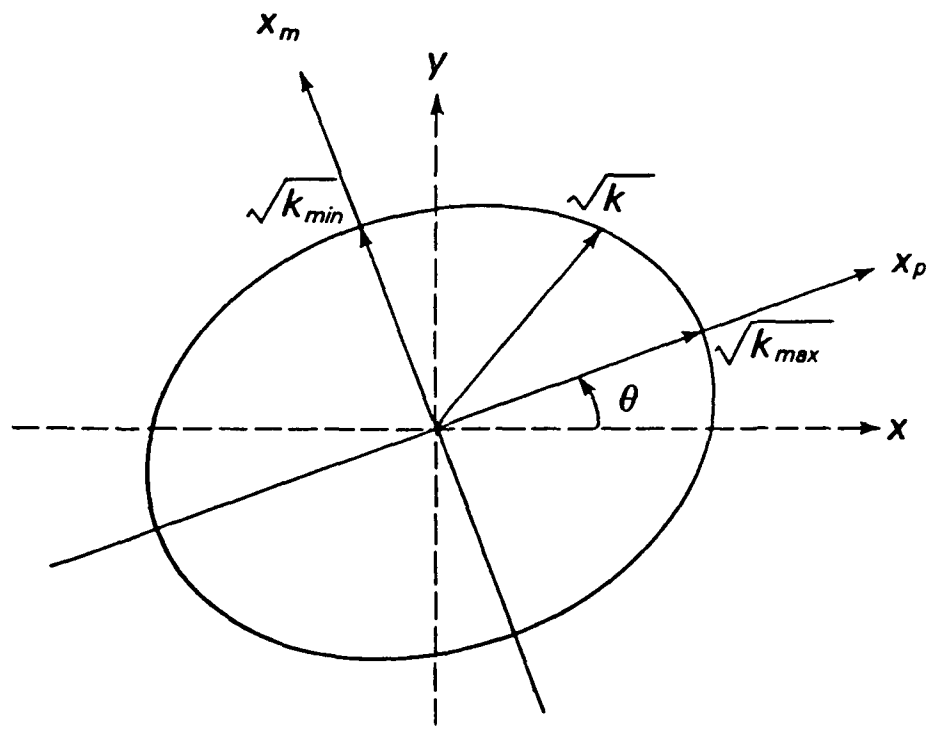


Figure 13. Definition of Anisotropic Permeability and Effective Permeability, k.

For most practical cases of solute transport:

$$\rho_o >> \left| \frac{d\rho}{dC} \right| C$$

so that:

$\rho \cong \rho_o$ = density of pure water.

d. Storativity

Specific pressure storativity, S_{op}, is defined as the volume of water and solute released from saturated pore storage due to a unit drop in fluid pressure in a representative aquifer volume VOL. This quantity can be expressed as:

$$S_{op} = (1 - \varepsilon)\alpha + \varepsilon\beta \tag{22}$$

where:

$$\alpha = -\frac{1}{VOL}\left[\frac{\partial(VOL)}{\partial\sigma'}\right]; \quad \beta = \frac{1}{\rho}\frac{\partial\rho}{\partial p}, \tag{23}$$

The physical quantities in these equations represent:

α = porous matrix compressibility,

β = coefficient of compressibility of water, and

σ' = effective intergranular stress.

A storativity defined in terms of a unit drop in piezometer head is denoted by S_o and has the units of m^{-1}. The relationship between S_o and S_{op} is given by:

$$S_o = \rho|\underline{g}|S_{op} = \rho g S_{op} . \tag{24}$$

e. Conservation of Fluid Mass

The conservation of fluid mass in a differential volume of an aquifer can be written as:

$$\underbrace{\frac{\partial}{\partial t}\left[\varepsilon S_w \rho\right]}_{\text{(storage)}} = \underbrace{-\underline{\nabla}\cdot\left[\varepsilon S_w \rho \underline{v}\right]}_{\text{(pore flow)}} + \underbrace{Q_p}_{\text{(fluid source)}} + \underbrace{T_p}_{\text{(solute source)}}, \tag{25}$$

where:

Q_p = net source/sink per cell, and

T_p = pure solute source/sink per cell.

However, the quantity T_p is usually assumed to be negligible in groundwater solute systems.

Equation (25) can be rewritten by invoking a series of assumptions and relationships, such as:

- By definition, $\frac{\partial(\varepsilon\rho)}{\partial p} = \rho S_{op}$
- Since C and T do not vary together, for convenience, U is taken to represent either C or T;
- Since (εS_w) is independent of C and T, $\frac{\partial\left[\varepsilon S_w\right]}{\partial U} = 0;$ (27)
- Darcy's Law holds;
- T_p is assumed to be zero.

After applying these conditions to Equation (25), the resultant conservation equation for unsaturated conditions is given by:

$$\left[S_w\rho S_{op} + \varepsilon\rho\frac{\partial S_w}{\partial p}\right]\frac{\partial p}{\partial t} + \left[\varepsilon S_w\frac{\partial\rho}{\partial u}\right]\frac{\partial U}{\partial t} - \underline{\nabla}\cdot\left[\left[\frac{\underline{\underline{k}}\, k_r\rho}{\mu}\right]\cdot\left[\underline{\nabla}p - \rho\underline{g}\right]\right] = Q_p \qquad (28)$$

For saturated flow ($S_w = 1$), Equation (28) simplifies to:

$$\rho S_{op}\frac{\partial p}{\partial t} + \varepsilon\frac{\partial\rho}{\partial U}\frac{\partial U}{\partial t} - \underline{\nabla}\cdot\left[\left[\frac{\underline{\underline{k}}\rho}{\mu}\right]\cdot(\underline{\nabla}p - \rho\underline{g})\right] = Q_p \qquad (29)$$

In both equations, the first term represents storage/pressure effects, the second term represents storage/concentration or temperature effects, the third term represents effects due to flow divergence, and the fourth term represents effects due to source/sinks.

2. Solute Transport Equations

a. Dispersion Tensor for Isotropic Media

For isotropic media, the dispersion tensor for both energy and solute balances is symmetric and second order:

$$\underline{\underline{D}} = \begin{bmatrix} D_{xx} & D_{xy} \\ D_{xy} & D_{yy} \end{bmatrix} \qquad (30)$$

where :

$$D_{xx} = \left[\frac{1}{v^2} \right] \left[d_L v_x^2 + d_T v_y^2 \right] \quad (31)$$

$$D_{yy} = \left[\frac{1}{v^2} \right] \left[d_T v_x^2 + d_L v_y^2 \right] \quad (32)$$

$$\underline{\underline{D}}_{xy} = \left[\frac{1}{v^2} \right] \left[d_L - d_T \right] \left[v_x \; v_y \right] \quad (33)$$

The quantities in Equations (31) to (33) are defined as:

$v_x(x,y,t)$ = magnitude of x-component of velocity

$v_y(x,y,t)$ = magnitude of y-component of velocity

$d_L(x,y,t)$ = longitudinal dispersion coefficient, and

$d_T(x,y,t)$ = transverse dispersion coefficient,

where:

$$v^2 = v_x^2 + v_y^2, \quad (34)$$

$$d_L = \alpha_L v, \text{ and} \quad (35)$$

$$d_T = \alpha_T v, \quad (36)$$

and where:

$\alpha_L(x,y)$ = longitudinal dispersivity of the soil matrix, and

$\alpha_T(x,y)$ = transverse dispersivity of the soil matrix.

A model of the flow-direction-dependent longitudinal dispersion is postulated in Figure 14. In this model, the longitudinal dispersivity is assumed to have two principal directions aligned with the principal directions of the permeability tensor, x_p and x_m. The principal values of longitudinal dispersivity in these directions are α_{Lmax} and α_{Lmin}. The dispersive flux components of the solute (or energy) in these principal permeability directions x_p and x_m are:

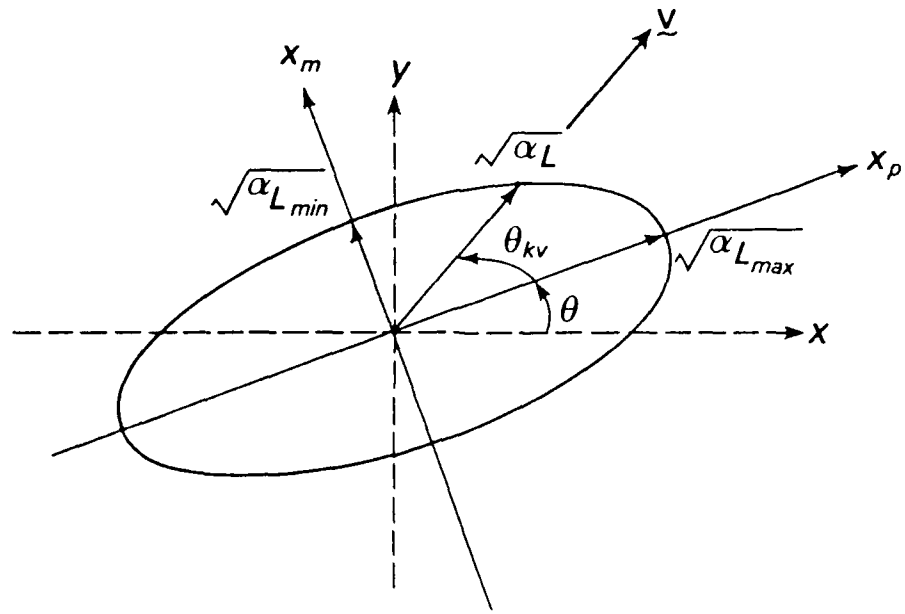


Figure 14. Definition of Flow-Direction-Dependent Longitudinal Dispersivity, $\alpha_L(\Theta)$.

$$F_p = -\alpha_{Lmax} \frac{\partial U}{\partial x_p} = F_s \cos(\Theta_{kv}) \quad (37)$$

$$F_m = -\alpha_{Lmin} \frac{\partial U}{\partial x_m} = F_s \sin(\Theta_{kv}) \quad (38)$$

where:

Θ_{kv} = angle from the maximum permeability direction to the local flow direction (see Figure 10).

The value of effective longitudinal dispersivity as dependent on the flow direction is given by:

$$\alpha_L = \frac{\left[\alpha_{Lmax}\right] \left[\alpha_{Lmin}\right]}{\left[\alpha_{Lmin} \cos^2(\Theta_{kv}) + \alpha_{Lmax} \sin^2(\Theta_{kv})\right]} \quad (39)$$

This expression is used by SUTRA to compute α_L for anisotropic media. Longitudinal dispersivity is adjusted for local anisotropy, while transverse dispersivity is assumed isotropic because it is generally smaller. Without a finer mesh, transverse dispersion anisotropy would be lost in discretization "noise". For isotropic media, $\alpha_{Lmax} = \alpha_{Lmin} = \alpha_L$.

b. Solute Adsorption

The adsorption of solute on the soil matrix is expressed as:

$$F = (1 - \varepsilon) \rho_s f_s \quad (40)$$

where:

f_s = specific solute mass adsorption rate per unit mass of solid matrix.

f = volumetric adsorbate source, or gain of adsorbed species by transfer from fluid per unit total volume.

ρ_s = density of solid grains in solid matrix (kg/m^3).

The units of f are solute mass per unit volume per second and those of f_s are solute mass per mass solid grains per second.

A general model for the specific solute adsorption rate f_s is given by:

$$f_s = k_1 \frac{\partial C}{\partial t} + k_2 C + k_3 , \quad (41)$$

where:

$$k_i = k_i (C, C_s), \qquad i = 1,2,3 , \tag{42}$$

and C_s is the adsorbate concentration on the surface of the soil grains. An example of a linear, reversible, nonequilibrium sorption model is as follows:

$$f_s = m_1 (C - m_2 C_s) \tag{43}$$

where m_1 and m_2 are sorption parameters. Equation (43) is of the form given in Equation (41) where $k_1 = k_2 = 0$ and $k_3 = m_1 C - m_1 m_2 C_3$.

Equilibrium sorption models are of the form of Equation (41) where $k_2 = k_3 = 0$, and where:

$$\frac{\partial C_s}{\partial t} = k_1 \frac{\partial C}{\partial t} \tag{44}$$

SUTRA considers three models of this type, namely:

(1) Linear isotherm

$$C_s = (X_1 \rho_o) C \tag{45}$$

where:

$$k_1 = X_1 \rho_o \tag{46}$$

(2) Freundlich isotherm

$$C_s = X_1 (\rho_o C)^{(1/X_2)} \tag{47}$$

where:

$$k_1 = (X_1/X_2) \rho_o^{(1/X_2)} C^{(1-X_2)/X_2} \tag{48}$$

(3) Langmuir isotherm

$$C_s = \frac{X_1 \rho_o C}{1 + X_2 \rho_o C} \tag{49}$$

where:

$$k_1 = \frac{X_1 \rho_o}{(1 + X_2 \rho_o C)^2} \tag{50}$$

Other model isotherms can be incorporated into the SUTRA code if the user prefers.

c. Solute and Adsorbate Production Terms

The production terms used in SUTRA for solute Γ_w and adsorbate Γ_s allow for first-order mass production (or decay) such as linear BOD (biochemical oxygen demand) or radioactive decay, biological or chemical production, and zero-order mass production (or decay). These source terms are given by:

$$\Gamma_w = \gamma_1^w C + \gamma_o^w \tag{51}$$

$$\Gamma_s = \gamma_1^s C + \gamma_o^s \tag{52}$$

where:

Γ_w = reaction source term per m^3 groundwater,

Γ_s = reaction source term per kg solid (matrix + adsorbate),

γ_1^w = first order reaction rate constant in aqueous phase (1/sec),

γ_1^s = first order reaction rate constant in adsorbed phase (1/sec),

γ_o^w = zero-order reaction rate constant in aqueous phase (kg_s/kg_w-sec), and

γ_o^s = zero-order reaction rate constant in adsorbed phase (kg_s/kg_g-sec).

d. Conservation of Solute

In an elemental volume of aquifer, the solute balance for the aqueous phase is:

$$\underset{\text{(storage)}}{\frac{\partial}{\partial t}\left[\varepsilon\rho S_w C\right]} = -f \underset{\text{(adsorption)}}{-} \underset{\text{(advection)}}{\underline{\nabla}\cdot\left[\varepsilon S_w \rho \underline{v} C\right]} + \underset{\text{(diffusion \& dispersion)}}{\underline{\nabla}\cdot\left[\varepsilon S_w \rho (D_M \underline{\underline{I}} + \underline{\underline{D}})\cdot\underline{\nabla} C\right]} + \underset{\text{(reaction)}}{\varepsilon S_w \rho \Gamma_w} + \underset{\text{(source/sink)}}{Q_p C^*} \tag{53}$$

where:

D_M = molecular diffusivity of solute in the aqueous phase,

$\underline{\underline{I}}$ = the identity tensor, and

C^* = solute concentration (mass fraction) in adsorbed phase.

The solute balance for the adsorbed phase in this elemental volume of aquifer is given by:

$$\underset{\text{(storage)}}{\frac{\partial}{\partial t}\left[(1-\varepsilon)\rho_s C_s\right]} = \underset{\text{(adsorption from aqueous phase)}}{f} + \underset{\text{(adsorption onto solid phase)}}{(1-\varepsilon)\rho_s \Gamma_s} \tag{54}$$

where:

C_s = specific concentration of adsorbate on solid grains [kg adsorbate/kg (grains + adsorbate)], and

Γ_s = reaction source term for solid phase [kg (adsorbate)/sec-kg (matrix + adsorbate)].

The conservation equation for the total solute over the elemental volume of aquifer is obtained by summing Equations (53) and (54). The result for unsaturated flow is:

$$\frac{\partial (\varepsilon S_w \rho C)}{\partial t} + \frac{\partial [\ (1-\varepsilon)\rho_s C_s\ ]}{\partial t} = - \underline{\nabla} \cdot \left[\varepsilon S_w \rho \underline{v} C \right] + \underline{\nabla} \cdot \left[\varepsilon S_w \rho \left(D_m \underline{\underline{I}} + \underline{\underline{D}} \right) \cdot \underline{\nabla} C \right] + \varepsilon S_w \rho \Gamma_w + (1 - \varepsilon)\rho_s \Gamma_s + Q_p C^* \tag{55}$$

For saturated flow, Equation (55) simplifies to:

$$\frac{\partial(\varepsilon\rho C)}{\partial t} + \frac{\partial[(1-\varepsilon)\rho_s C_s]}{\partial t} = - \underline{\nabla} \cdot (\varepsilon\rho \underline{v} C) + \underline{\nabla} \cdot (\varepsilon\rho \underline{v} C) + \underline{\nabla} \cdot \left[\varepsilon\rho (D_m \underline{\underline{I}} + \underline{\underline{D}}) \cdot \underline{\nabla} C \right] + \varepsilon\rho\Gamma_w + (1-\varepsilon)\rho_s \Gamma_s + Q_\rho C^* \tag{56}$$

For saturated flow without adsorption:

$$\frac{\partial(\varepsilon\rho C)}{\partial t} = - \underline{\nabla} \cdot (\varepsilon\rho \bar{\underline{v}} C) + \underline{\nabla} \cdot \left[\varepsilon\rho (D_m \underline{\underline{I}} + \underline{\underline{D}}) \cdot \underline{\nabla} C \right] + \varepsilon\rho\Gamma_w + Q_p C^* \tag{57}$$

3. Energy Transport Equation

The conservation of energy equation for saturated flow conditions is analogous to that for the conservation of total solute, Equation (56). Thus, in terms of the water/solute/soil matrix temperature T, the equation is given as:

$$\underbrace{\frac{\partial}{\partial t} \left[[\varepsilon\rho c_w + (1-\varepsilon)\rho_s c_s]\ T \right]}_{\text{(aqueous storage absorption)}} + \underbrace{\underline{\nabla} \cdot \left[\varepsilon\rho c_w \underline{v} T \right]}_{\text{(advection)}} - \underbrace{\underline{\nabla} \cdot \left[[\varepsilon\tau_w + (1-\varepsilon)\tau_s] \underline{\underline{I}} + \varepsilon\rho c_w \underline{\underline{D}} \right]}_{\text{(dispersion)}} = \underbrace{Q_p c_w T^*}_{\text{(fluid source)}} + \underbrace{\varepsilon\rho\gamma_o^w}_{\text{(aqueous phase energy source)}} + \underbrace{(1-\varepsilon)\rho_s \gamma_o^s}_{\text{(adsorbed phase energy source)}} \tag{58}$$

where:

τ_s = thermal conductivity of solid matrix,

τ_w = thermal conductivity of fluid,

c_w = specific heat of water,

c_s = specific heat of solid matrix,

$\underline{\underline{D}}$ = thermal dispersion tensor,

T^* = temperature of source fluid,

γ_o^w = energy source in fluid, and

γ_o^w = energy source in solid grains.

C. SUTRA'S FINITE ELEMENT MESH

SUTRA is a hybrid of finite element analysis (used for flux terms), and integrated finite difference analysis (used for nonflux terms). Finite element analysis provides mathematical elegance and geometric flexibility, while integrated finite difference method provides computational efficiency. Parametric values are optimized using matrix algebra and the method of weighted residuals. A symmetric function is usually chosen for weighting. However, an asymmetric weighting function is available when required for simulations with strong convection effects or for simulating unsaturated flows. The method of evaluation of velocity and pressure was designed to minimize numerical dispersion.

1. Aquifer Discretization

An aquifer is a three-dimensional region, but SUTRA performs a two-dimensional analysis. So, SUTRA divides the aquifer into a single layer of contiguous blocks called finite elements. Each hydrologic unit in the aquifer is divided into many such elements. Thus, the aquifer takes on the appearance of a "fine net" or "mesh." The basic building block of the mesh is a finite element, which is a quadrilateral with a finite length and width, and a depth equal to the full aquifer thickness (Figure 15).

There are a number of restrictions on the mesh. All twelve edges of an element must be perfectly straight. Four edges are parallel to the z axis*. The xy-plane bisects each of these four edges, so the top and bottom surfaces of an element are mirror images of each other. An aquifer thickness is specified at each node. The nodes are located where the z edges of the elements intersect the xy-plane. The xy-plane may be inclined to the horizontal; however, the plane must not be folded or warped. Each element has four nodes, and except at the edges of the aquifer or at pinch nodes, each node is shared with three other elements. Aquifer parameters may vary in the x and y dimensions, but not with z.

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* All references to axes in this paragraph pertain to an areal flow mesh. For vertical cross-sectional or vertical radial meshes, substitute the analogous axes.

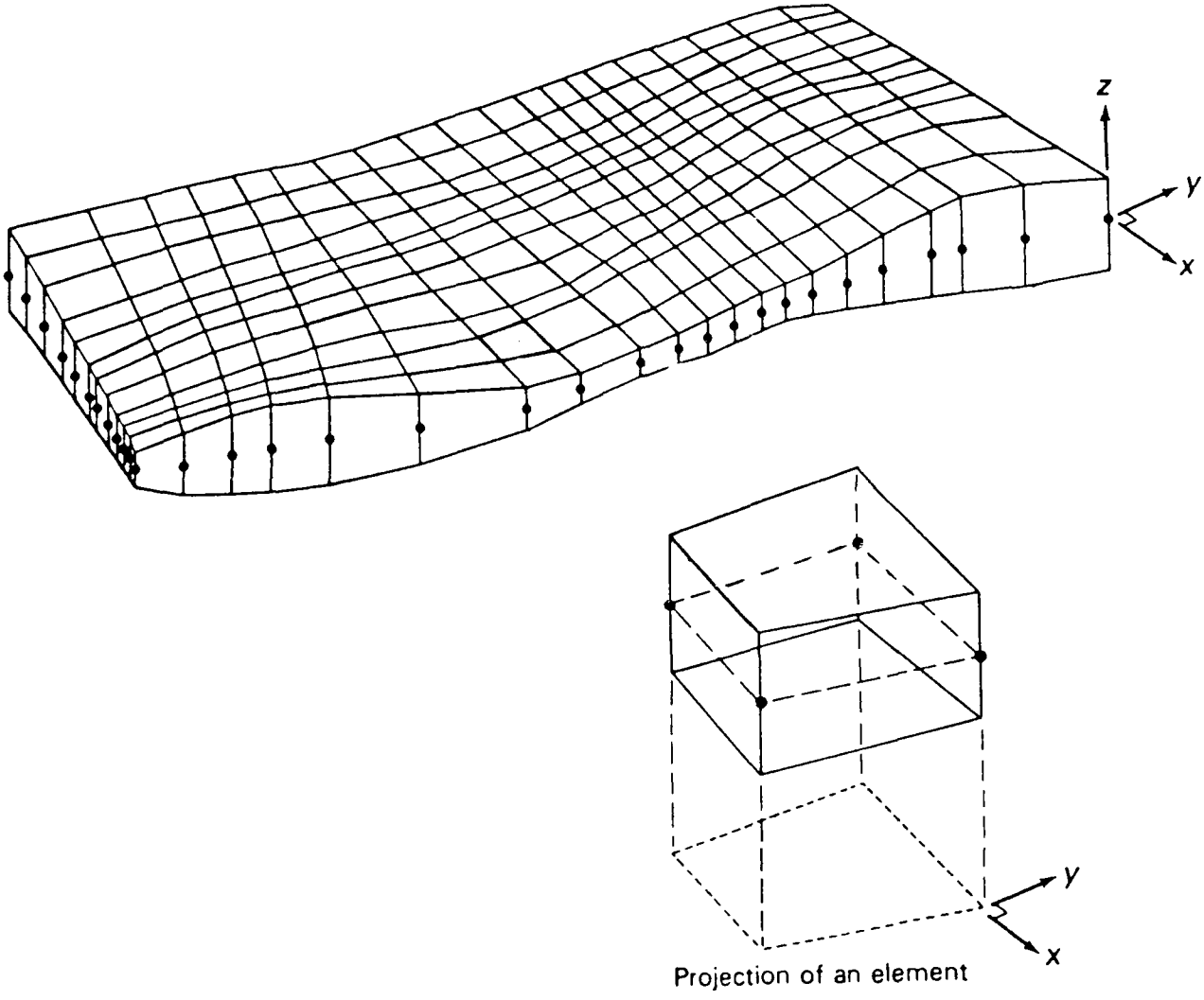

Figure 15. Two-Dimensional Finite-Element Mesh and Quadrilateral Element (Reference 8).

While aquifer properties and parameters may actually behave as continuous variables, SUTRA specifies them discretely in three ways*: by element, by cell, and by node. A parameter discretized by element is shown in Figure 16; note the appearance of the flat-topped boxes. Each parametric value is constant within each element. For example, hydraulic conductivity and dispersivity are specified by element. Discretization by cell is analogous to discretization by element, but is centered on nodes, rather than on the centers of elements (Figure 17). Storativity and $(\partial h/\partial t)$ are specified by cells.

The third type of specification is by node (Figure 18). The user specifies values only at nodes, but SUTRA can calculate intermediate values by using "basis functions" to interpolate, performing a 2-D, 4-point bilinear interpolation. Head, temperature, and concentration are discretized by node.

SUTRA basis functions are bilinear in terms of local coordinates $\xi = \xi(x,y)$ and $\eta = \eta(x,y)$, where (x,y) ranges over the physical domain of interest (i.e., the global coordinates) and where (ξ, η) ranges over the square defined by $-1 \le \xi \le 1$ and $-1 \le \eta \le 1$. The coordinate mapping, $\xi(x,y)$ and $\eta(x,y)$, from the global coordinates to the local coordinates is linear and each element in the physical domain is mapped into the square (i.e, $-1 \le \xi \le 1$, $-1 \le \eta \le 1$) in the local coordinates (Figure 19). Thus, the functional relationships given by:

$$\begin{aligned} \xi &= \xi(x,y) \\ \eta &= \eta(x,y) \end{aligned} \tag{59}$$

vary from element to element over the physical domain of computation.

Over the image of each physical element (Figure 19B), there are four basis functions defined, one for each quadrant:

$$\begin{aligned} \Omega_1(\xi,\eta) &= \Xi_-H_- & \Omega_2(\xi,\eta) &= \Xi_+H_- \\ \Omega_3(\xi,\eta) &= \Xi_+H_+ & \Omega_4(\xi,\eta) &= \Xi_+H_+ \end{aligned} \tag{60}$$

The numerical subscripts refer to the numbered nodes in Figure 19. As indicated by Equation (60), each of the above basis functions is the product of two one-dimensional basis functions:

$$\begin{aligned} \Xi_-(\xi) &= 1/2\ (1-\xi) & \Xi_+(\xi) &= 1/2\ (1+\xi) \\ \Xi_-(\eta) &= 1/2\ (1-\eta) & \Xi_+(\eta) &= 1/2\ (1+\eta) \end{aligned} \tag{61}$$

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* However, simulation control parameters, adsorption parameters, and reaction parameters are assumed constant throughout the aquifer. And provided temperature and concentration effects are small, fluid properties will be constant, as well.

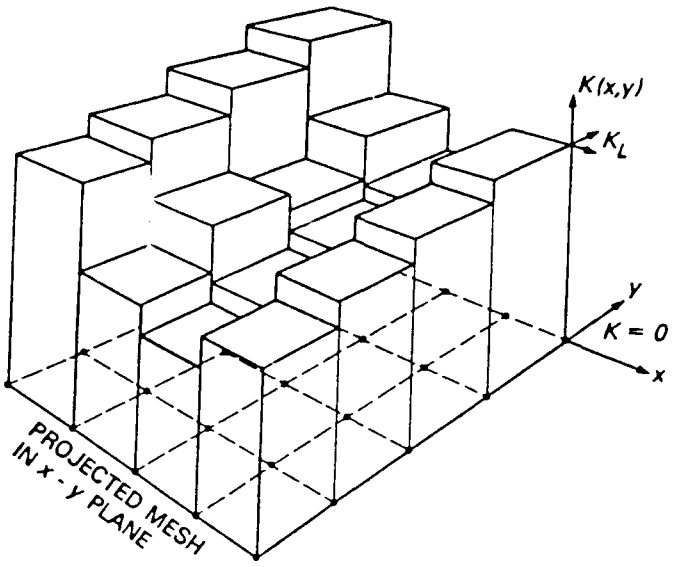

Figure 16. Discretization (by Element) of Coefficient K(x,y) (Reference 8).

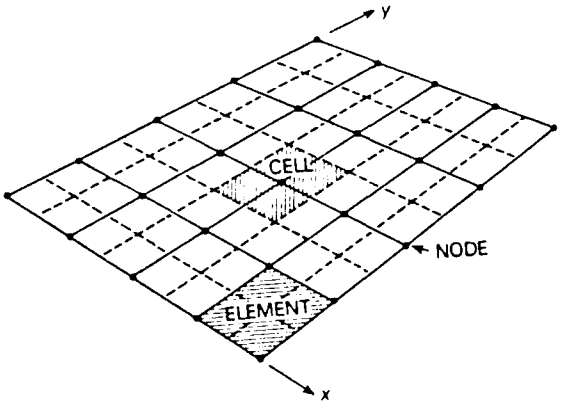

Figure 17. Cells, Elements and Nodes for a Two-Dimensional Finite-Element Mesh Composed of Quadrilateral Elements (Reference 8).

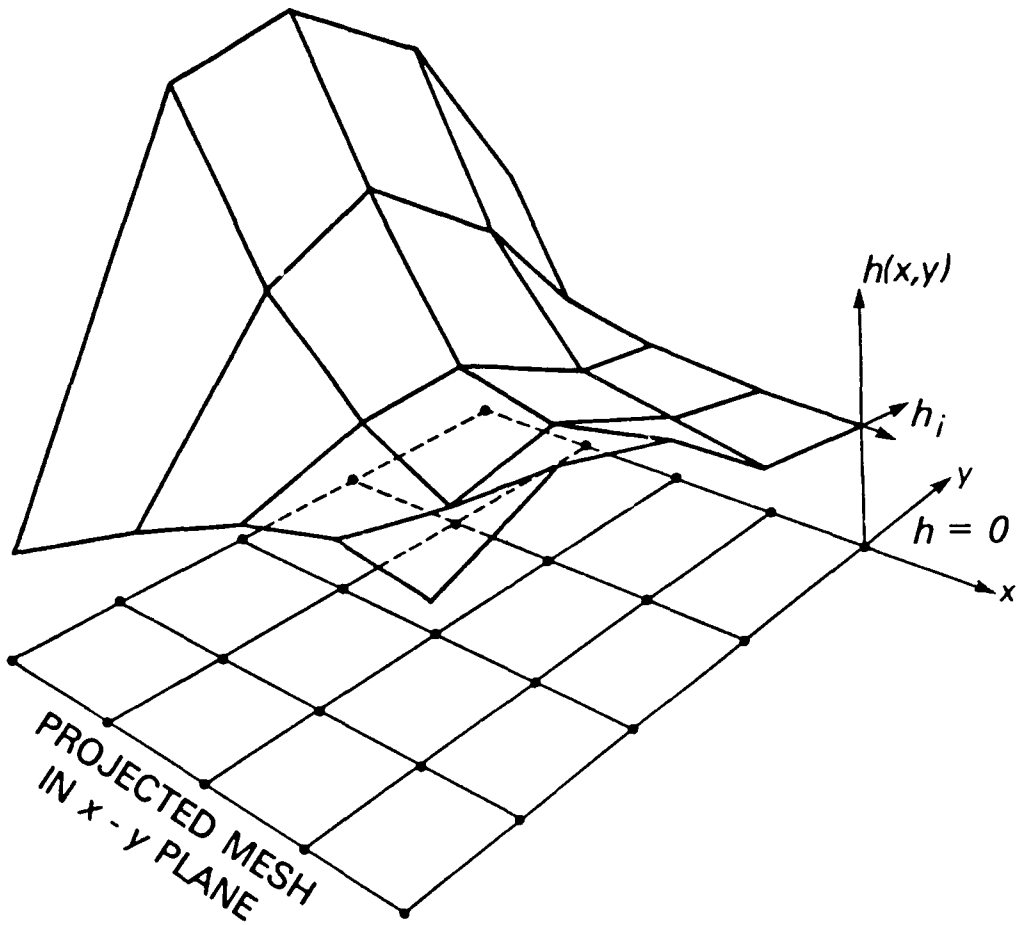

Figure 18. Nodewise Discretization of Coefficient h(x,y).

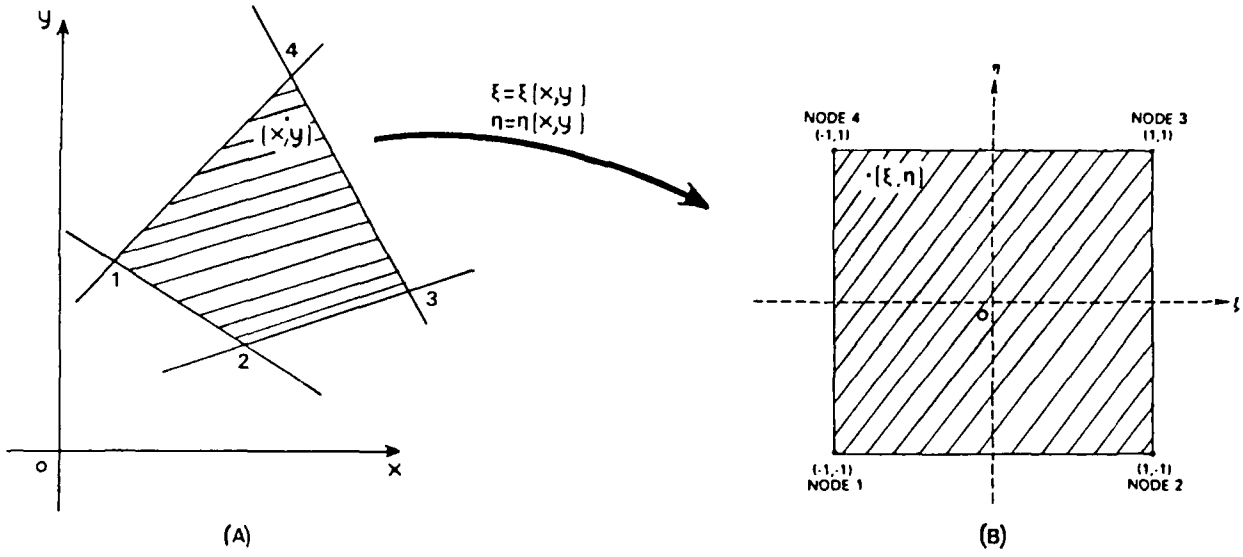

Figure 19. Transformation from a Finite Element in Physical Space (i.e., the Global Coordinates in Figure A) to a Square Element (Figure B) in the Local Coordinates (After Reference 8).

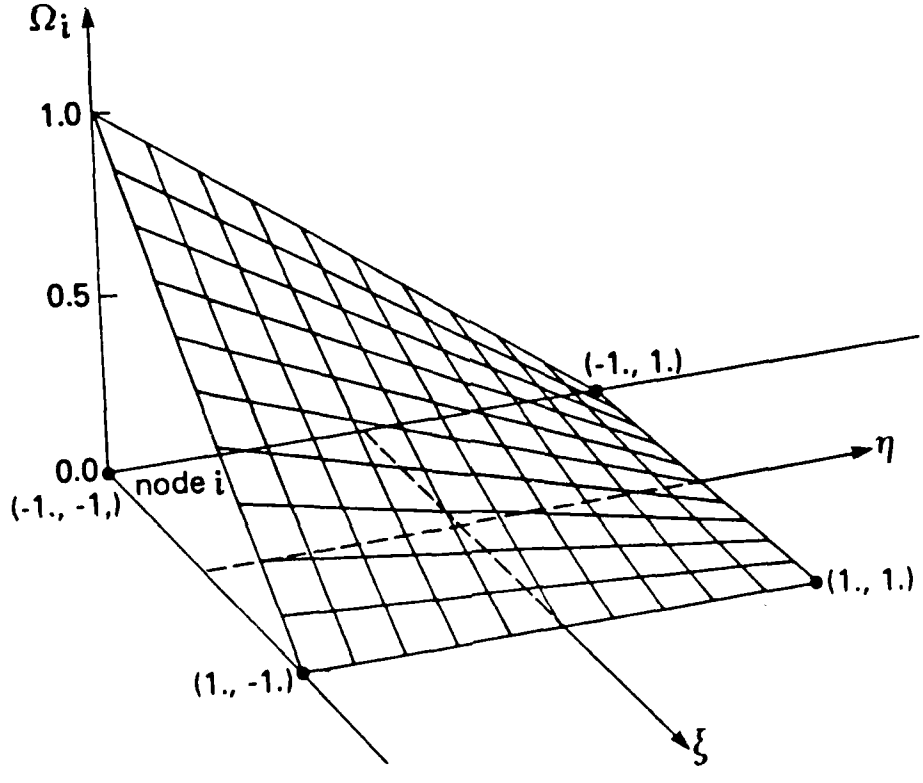

Figure 20. Perspective of Basis Function Ω_i (,η) at Node i (Reference 8).

Figure 20 shows a three-dimensional plot of the 2-D basis functions over one element. Note how the plotted surface lends itself to bilinear interpolation. Note also that each basis function (Ω_1 to Ω_4) has a value of 1 at its own node and zero at the other three nodes.

Pinch nodes are an option that may be used to facilitate abrupt changes in mesh size. Some parts of a mesh may be "busier" than others, and may require a finer mesh. With pinch nodes, some rows or columns of elements may be partially subdivided, permitting a mesh with fewer elements than if those rows and columns were fully subdivided (Figure 21). However, the use of pinch nodes increases matrix bandwidth. At present, the matrix solver algorithm depends on bandwidth. So while pinch nodes reduce the number of elements, the speed of solution is nearly unaffected. In the future, a new bandwidth-independent matrix solver algorithm may be added to take full advantage of the pinch-node capability.

2. Weighting Functions

The choice of weighting functions can affect mesh size. Weighting functions are used in calculating integral expressions. The Galerkin method calculates weighted integrals, and adjusts certain parameters to force the weighted integrals close to zero in all parts of the aquifer. Normally, the symmetric Galerkin "weighting function" is used. This is the default case. In some cases, however, the discretization is too coarse to properly represent the actual advection and dispersion, so the use of an asymmetric weighting function is helpful. Here, the Galerkin-Petrov method with its asymmetric weighting function may be substituted.

Asymmetric weighting is specified by an input parameter, GNUO, the "upstream weighting factor," which controls the degree of asymmetry. This factor varies continuously from zero, pure symmetric weighting, to 1, fully asymmetric weighting. Simulating unsaturated flows is a major use of asymmetric weighting. In most cases, however, the asymmetric function adds too much numerical dispersion, and symmetric basis function are preferred.

SUTRA allows its quadrilateral elements to have an arbitrary shape, provided the sides are straight (Figure 19A). This advantage is possible because of the built-in coordinate transformation algorithms. The node positions (and element coordinates) are specified in "global coordinates." Any mathematical operations that use basis (or weighting) functions, such as volume integration or Gaussian integration, are performed in "local coordinates," with each element as a 2 unit x 2 unit (dimensionless) square, centered at the origin (Figure 19B). The transformation to local coordinates involves the Jacobian matrix of the transformation equations shown in Figure 19, and transformation back to global coordinates uses the corresponding inverse Jacobian matrix (see pp. 100-102 of Reference 8).

D. NUMERICAL APPROXIMATION OF BALANCE EQUATIONS

1. Groundwater Flow Equation

The conservation of mass equation for a soil fluid under unsaturated conditions can be written as (Equation 28):

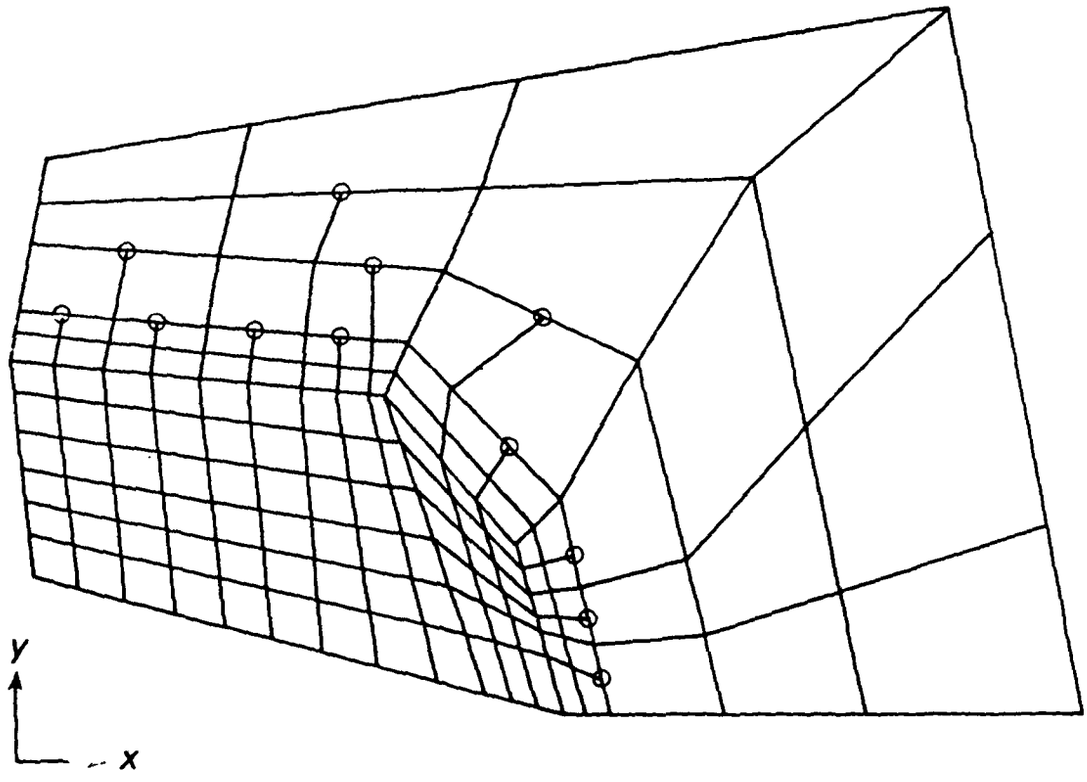

Figure 21. Finite-Element Mesh with Pinch Nodes.

$$O_p(p,U) = 0 \tag{62}$$

where $O_p(p,U)$ represents the following expression:

$$\left[S_w \rho S_{op} + \varepsilon \rho \frac{\partial S_w}{\partial p} \right] \frac{\partial p}{\partial t} + \left[\epsilon S_w \frac{\partial \rho}{\partial U} \right] \frac{\partial U}{\partial t} - \underline{\nabla} \cdot \left[\left[\frac{\underline{\underline{k}}\, k_r \rho}{\mu} \right] \cdot \left[\underline{\nabla} p - \rho \underline{g} \right] \right] - Q_p - \nu_p \rho g \left[h_{BC} - h \right] \tag{63}$$

The quantity $\nu_p \rho g(h_{BC} - h)$ represents the specified head boundary conditions which have been separated from the other boundary conditions, represented by Q_p. As illustrated in Figure 22, ν_p is the flow conductance of the aquifer boundary at the source node i, and h_{BC} is the external head of the source.

The quantity $O_p(p,U)$ is identically zero over the physical domain of interest if all pnysical parameters are properly specified and the pressure p and the dependent variable U are known exactly. However, because of the complexity of the terms in Equation (63) and in the other conservation equations, these parameters and dependent variables are rarely known to a degree required to satisfy Equation (62). Hence, $O_p(p,U)$ must be discretized by node, by cell, and/or by element, which leads to an approximation of Equation (62) given by:

$$O_p(p,U) = R_p(x,y,t) \tag{64}$$

where $R_p(x,y,t)$ is generally a nonzero, spatially varying residual and the symbol indicates that the terms beneath it are discretized in one or more of the three methods.

a. Spatial Integration

If the proper global-coordinate weighting function $W_i(x,y)$ is chosen, then the volume integral of Equation (64) over the physical domain of interest V becomes

$$\int_V O_p(p,U) \; W_i(x,y) \; dV = 0 \;, \tag{65}$$

where the subscript i represents elements, cells, and/or nodes, depending on the method of discretization. The index i ranges from 1 to an integer dependent on the N x N mesh, denoted by $i = \overline{1,NN}$.

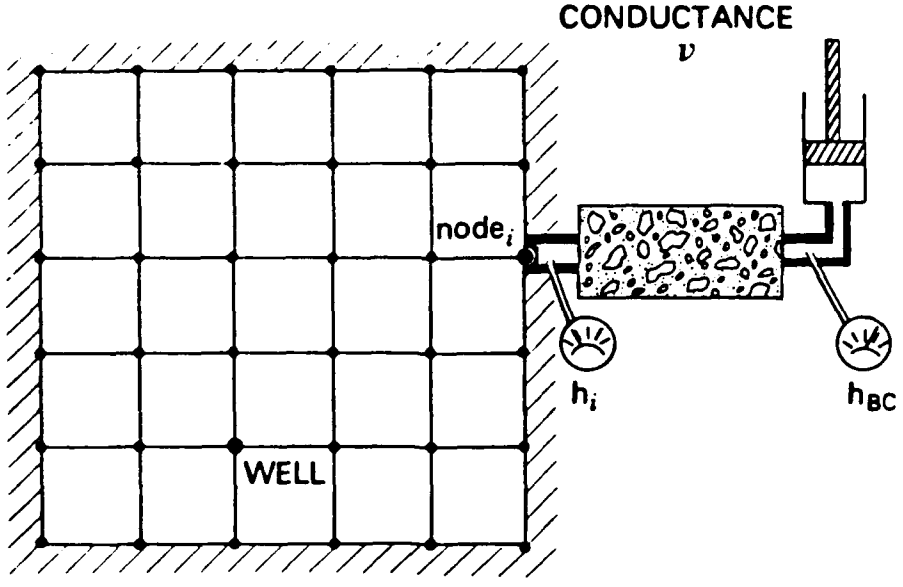

Figure 22. Schematic Representation of Specified Head or Pressure (Reference 8).

Applying the proper discretization to the terms in Equation (63) as discussed in Section IV-C, applying various classical integral theorems and numerical algorithms, and using convenient weighting functions (see Reference 8), Equation (65) can be rewritten as:

$$AF_i \frac{dp_i}{dt} + CF_i \frac{dU_i}{dt} + \sum_{j=1}^{NN} p_j(t)\, BF_{ij} + \nu_i p_i = Q_i + \nu_i p_{BC} + q_{In_i} + DF_i \qquad (66)$$

where $i = \overline{1,NN}$, V_i = volume of cell i, $\hat{\underline{\underline{k}}}^L$ = the discretization of $\underline{\underline{k}}$ by element, $\varphi_i(x,y)$ = a basis function, $W_i(x,y)$ = asymmetric weighting function, and $(\rho^* g)$ = discretization of (ρg) consistent with the discretization of $\underline{\nabla}p$, and where

$$AF_i = \left[S_w \rho S_{op} + \varepsilon\rho \frac{\partial S_w}{\partial p} \right] i \cdot V_i \qquad (67)$$

$$CF_i = \left[\varepsilon S_w \frac{\partial \rho}{\partial U} \right] i \cdot V_i \qquad (68)$$

$$BF_{ij} = \int_x \int_y \left\{ \left[\left[\hat{\underline{\underline{k}}}^L \right] \left[\frac{\hat{k}_r \rho}{\mu} \right] \right] \cdot \underline{\nabla} \varphi_j \right\} \cdot \underline{\nabla} w_i \; B \; dy \; dx \qquad (69)$$

$$DF_i = \int_x \int_y \left\{ \left[\hat{\underline{\underline{k}}}^L \left[\frac{\hat{k}_r \rho}{\mu} \right] \right] \cdot \left[\hat{\rho}^* g \right] \right\} \cdot \underline{\nabla} w_i \; B \; dy \; dx \qquad (70)$$

Equation (66) represents a system of ordinary differential equations which are nonlinear and coupled with respect to the time-dependent unknowns. The quantities BF_{ij} and DF_i require Gaussian integration (discussed in Section IV-D-3) and are evaluated in an element-by-element manner, while AF_i and CF_i are evaluated by cell.

b. Time Discretization

The time derivative of pressure p is given by:

$$\frac{dp_i}{dt} \simeq \frac{p_i^{n+1} - p_i^n}{\Delta t_{n+1}} \qquad (71)$$

where:

$$p_i^n = p_i(t^n) \quad , \qquad (72)$$

$$p_i^{n+1} = p_i \left[t^n + \Delta t_{n+1} \right] = p_i \left[t^{n+1} \right] , \tag{73}$$

$$\Delta t_{n+1} = t^{n+1} - t^n , \tag{74}$$

and where the superscript involving (n) or (n+1) indicates the level of time evaluation.

Terms with level (n+1)* indicate that the terms are evaluated at the n^{th} time level on a first iteration, and at the most recent time level on subsequent iterations. Since dU_i/dt only contributes a small amount to the balance given in Equation (66), it is approximated by:

$$\frac{dU}{dt} \simeq \left[\frac{dU_i}{dt} \right]^n = \frac{U_i^n - U_i^{n-1}}{\Delta t_n} \tag{75}$$

The final form of the time-discretized Equation (66) (i.e., the system implemented in SUTRA) is as follows:

$$\sum_{j=1}^{NN} \left[\frac{AF_i \ \delta_{ij}}{\Delta t_{n+1}} + BF_{ij}^{n+1} + \nu_i \delta_{ij} \right] p_j^{n+1} = Q_i^{n+1} + \nu_i p_{BC_i}^{n+1} + DF_i^{(n+1)^*} + \left[\frac{AF_i^{n+1}}{\Delta t_{n+1}} \right] p_i^n + \left[CF_i^{n+1} \right] \left[\frac{dU_i}{dt} \right]^n , \tag{76}$$

where $\overline{i = 1, NN}$ and where δ_{ij} is the Kronecker delta given by:

$$\delta_{ij} = \begin{cases} 0 \text{ if } i \neq j \\ 1 \text{ if } i = j \end{cases} . \tag{77}$$

Because the coefficients in Equation (76) depend on the unknown values of p and U at the end of the time step (t^{n+1}), one or more iterations may be used to solve this nonlinear problem. On the first iteration, and when only one iteration per time step is used, the coefficients are based on a time-projected values of p and U, namely:

$$p_i^{proj} = p_i^n + \left[\frac{\Delta t_{n+1}}{\Delta t_n} \right] \left[p_i^n - p_i^{n-1} \right] \tag{78}$$

$$U_i^{proj} = U_i^n + \left[\frac{\Delta t_{n+1}}{\Delta t_n} \right] \left[U_i^n - U_i^{n-1} \right] \tag{79}$$

These projections estimate the p and U values at a node i, p_i^{proj} and U_i^{proj}, at the end of the present time step, Δt_{n+1}, based on linear extrapolation of the two previous values of p and U. All p and U dependent coefficients in Equation (76) are estimated at time level t^{n+1}. These coefficient values are based on the most recent values of p and U, be they projections or solutions to the previous iteration. Iterations end when the maximum change in p and U at any node in the mesh falls below user-specified criteria of absolute change in p and U.

c. Boundary Conditions and Source/Sink Terms

Specified node pressures, which may change with each time step, are listed by cell in the boundary conditions, and are maintained by the addition of a fluid fluxes, Q_{BC_i} (kg/sec), expressed as:

$$Q_{BC_i}^{n+1} = \nu_{p_i} \left[p_{BC_i}^{n+1} - p_i^{n+1} \right] \qquad (80)$$

This was illustrated in Figure 22. For a cell in which ν_{p_i} is specified as a large number,

$$p_{BC_i}^{n+1} \cong p_i^{n+1} \; . \qquad (81)$$

For cells in which a pressure boundary condition is not specified, ν_{p_i} is set equal to zero, and no fluid is added to the cell by this boundary condition.

Both fluid sources and sinks that flow across aquifer boundaries at specified rates are accounted for by the vector Q_i^{N+1} in Equation (76) and are generically referred to as fluid sources.

2. Solute/Energy Transport Equations

Because of the structural similarities between the SUTRA solute and energy transport balances, it is convenient to represent them in the source code with a common equation:

$$\underbrace{\left[\varepsilon S_w \rho c_w + (1-\varepsilon)\, \rho_s c_s \right] \frac{\partial U}{\partial t}}_{\text{(storage)}} + \underbrace{\varepsilon S_w \rho c_w \underline{v} \cdot \underline{\nabla} U}_{\text{(advection)}}$$

$$- \underline{\nabla} \cdot \left\{ \underbrace{\rho c_w \left[\varepsilon s_w \left(\sigma_w \underline{\underline{I}} + \underline{\underline{D}} \right) + (1-\varepsilon) \sigma_s \underline{\underline{I}} \right]}_{\text{(dispersion)}} \cdot \underline{\nabla} U \right\} =$$

$$Q_p c_w (U^* - U) + \varepsilon S_w \rho \gamma_1^w U + (1-\varepsilon)\rho_s \gamma_1^s U_s + \varepsilon S_w \rho \gamma_o^w + (1-\varepsilon)\rho_s \gamma_o^s + \qquad (82)$$

(external sources (constant flux)) (aqueous phase) (energy source terms) (adsorbed phase)

$$Q_{PBC} c_w (U_{BC} - U),$$

(energy transported by constant head sources)

where for energy transport:

$$U \equiv T,\ U_s = c_s T,\ U^* \equiv T^*,\ \sigma_w \equiv \frac{\tau_w}{\rho c_w},\ \sigma_s \equiv \frac{\tau_s}{\rho c_w},\ \gamma_1^w \equiv \gamma_1^s \equiv 0,$$
$$\Gamma_w = \gamma^o,\ \Gamma_s = \gamma_s^o \qquad (83)$$

and for solute transport

$$U \equiv C,\ U_s \equiv C_s,\ U^* \equiv C^*,\ \sigma_w \equiv D_m,\ \sigma_s \equiv 0,\ c_w \equiv 1,\ c_s = k_1 \qquad (84)$$

The quantity C_s is defined by Equation (45), (47), or (49), and k_1 is given by Equation (46), (48), or (50), depending on the isotherm used in the SUTRA simulation. The quantity Q_{PBC} is the mass fluid source rate and U_{BC} is the concentration or temperature of the flow from this source. For outflow $U_{BC} = U$, and the last term in Equation (82) goes to zero.

The form of the fluid mass/energy/species balance equation given by Equation (82) is the system implemented in SUTRA using the weighted-residual numerical approximation. In this formulation, Equation (82) is abbreviated by

$$O_u(U) = 0, \qquad (85)$$

where $O_u(U)$ represents the following terms:

$$\left[\varepsilon S_w \rho c_w + (1-\varepsilon)\rho_s c_s \right] \frac{\partial U}{\partial t} + \varepsilon S_w \rho c_w \underline{v} \cdot \underline{\nabla} U$$
$$- \underline{\nabla} \cdot \left\{ \rho c_w \left[\varepsilon S_w (\sigma_w \underline{\underline{I}} + \underline{\underline{D}}) + (1-\varepsilon)\sigma_s \underline{\underline{I}} \right] \cdot \underline{\nabla} U \right\}$$
$$- Q_p c_w (U^* - U) - \varepsilon S_w \rho \gamma_1^w U - (1-\varepsilon)\rho_s \gamma_1^s U_s - \varepsilon S_w \rho \gamma_o^w - (1-\varepsilon)\rho_s \gamma_o^s \qquad (86)$$
$$- Q_{QBC} c_w (U_{BC} - U).$$

a. Spatial Integration of Equation (85)

The approximation of $O_u(U) = 0$ through discretization by node, element, and/or cell results in the system

$$O_u(U) = R_u(x,y,t), \tag{87}$$

where R_u is the nonzero residual due to the discretization process. Using weighting functions $W_i(x,y)$ and integrating Equation (87) over the domain of computation V, gives

$$\int_V O_u(U) \; W_i(x,y) \; dV = 0 \; . \tag{88}$$

Using theorems, relationships, and discretized approximations similar to those used for Equation (65), allows Equation (88) to be reduced to the following nonlinear, coupled set of ordinary differential equations:

$$AT_i \frac{dU_i}{dt} + \sum_{j=1}^{NN} U_j(t) \; DT_{ij} + \sum_{j=1}^{NN} U_j(t) \; BT_{ij} - \left[GT_i + G_s TL_i \right] U_i(t) \tag{89}$$

$$+ Q_i \, c_w \, U_i(t) + Q_{BC_i} c_w \, U_i(t) = Q_i c_w U_i^* + Q_{BC_i} c_w U_{BC_i} + \Psi_{IN_i} + ET_i + G_s TR_i$$

where $\overline{i = 1,NN}$ and where:

$$AT_i = \left[\varepsilon S_w \rho c_w + (1-\varepsilon)\rho_s c_s \right]_i V_i \tag{90}$$

$$DT_{ij} = \int_x \int_y \left[\hat{\varepsilon}(S_w \rho) c_w \hat{\underline{v}}^* \cdot \underline{\nabla} \varphi_j \right] \omega_i \; B \; dy \; dx \tag{91}$$

$$BT_{ij} = \int_x \int_y \left[\rho c_w \left[\hat{\varepsilon} S_w \left(\sigma_w \underline{\underline{I}} + \hat{\underline{\underline{D}}} \right) + (1-\hat{\varepsilon}) \sigma_s \underline{\underline{I}} \right] \cdot \underline{\nabla} \varphi_j \right] \cdot \underline{\nabla} \varphi_i \; B \; dy \; dx \tag{92}$$

$$GT_i = \left[\varepsilon S_w \rho \gamma_1^w \right]_i V_i \tag{93}$$

$$G_s TL_i = \left[(1-\varepsilon)\rho_s \gamma_1^s \, s_L \right]_i V_i \tag{94}$$

$$G_s TR_i = \left[(1-\varepsilon)\rho_s \gamma_1^s \, s_R \right]_i V_i \tag{95}$$

$$ET_i = \left[\varepsilon s_w \rho \gamma_o^w + (1-\varepsilon)\rho_s \gamma_o^s \right]_i V_i \tag{96}$$

The integrals BT_{ij} and DT_{ij} require Gaussian integration (see Section IV-D-3) and are evaluated in an element-by-element fashion. The remaining terms that do not involve Q_{BC} are evaluated cell-by-cell in subroutine SUTRA. The flux terms arising from the specified pressure (those containing Q_{BC}) are evaluated by subroutine BCB (see Section IV-D-2-c).

b. Time Discretization

The time derivatives in Equation (89) are discretized in the same way as in Section IV-D-1-b, resulting in the following NN spatially and temporally discretized system:

$$\sum_{j=1}^{NN}\left\{\left[\frac{AT_i^{n+1}\ \delta_{ij}}{\Delta t_{n+1}}\right] + DT_{ij}^{(n+1)^*} + BT_{ij}^{n+1} + \left[GT_i^{n+1} + G_s TL_i^{n+1} + \left(Q_i^{n+1} + Q_B^{(n+1)^*}\right)c_w\right]\right.$$

(97)

$$\left.\delta_{ij}\right\} U_i^{n+1} = c_w\left[Q_i^{n+1}\ U_i^{(n+1)^*} + Q_{BC_i}^{n}\ U_{BC_i}^{n+1}\right] + \Psi_{IN_i}^{n+1} + ET_i^{n+1} + G_s TR_i^{n+1} + \left[\frac{AT_i^{n+1}}{\Delta t_{n+1}}\right] U_i^n$$

where δ_{ij} is the Kronecker delta and $i = \overline{1, NN}$

The $(n+1)^*$ level indicates that velocity and Q_{BC} are evaluated on the first iteration at the time step (n) and on subsequent iterations, at the most recent level. Other coefficients in Equation (97) are evaluated at the (n+1) time level by projection on the first iteration, and then at the most recent level on subsequent iterations.

c. Boundary Conditions and Fluid Sources and Sinks

A specified temperature or concentration boundary condition is obtained numerically at a specified node k by replacing the k^{th} equation in Equation 89 by:

$$U_k^{n+1} = U_{BC_k}^{n+1} \tag{98}$$

where $U_{BC_k}^{n+1}$ is a user-specified value of U at node k during time step (n+1). This specified value may change with each time step.

Source boundary conditions for U may arise at points of specified pressure when an inflow Q_{BC_i} occurs at such a point. A value of U must be specified for these fluid inflows, denoted as $U_{BC_i}^{n+1}$. These values may change with each time step.

Specified pressures are maintained at a cell by the addition of fluid from a source or fluid leakage to a sink as shown in Equation 80. The quantity $\Psi_{IN_i}^{n+1}$ represents a source or sink at a boundary due to diffusion or dispersion. It is defined by the surface integral:

$$\Psi_{IN_i}^{n+1} = \int_{\Gamma} \left[\rho c_w \left\{ \varepsilon s_w \left(\sigma_w \underline{\underline{I}} + \underline{\underline{D}} \right) + (1-\varepsilon)\, \sigma_s \underline{\underline{I}} \right\} \cdot \underline{\nabla U} \right]^{n+1} \cdot \underline{n}\, \varphi_i \, d\Gamma \qquad (99)$$

The quantity $\Psi_{IN_i}^{n+1}$ is a heat or solute flux, and is entered in the input data file as a user-specified value, which may change with each time step. If the term is set to zero, it implies no diffusion and no dispersion across a boundary for solute transport. For energy transport, zero implies perfect thermal insulation and no dispersion across a boundary. For an open boundary across which fluid flows, the quantity is not automatically evaluated by SUTRA. If no user-specified value exists at an open boundary, then this term is set to zero. This implicitly assumes that the largest part of solute or energy flux across an open boundary is advectively transported rather than diffusively or dispersively transported.

3. Gaussian Integration

Several integral terms in Equations (76) and (97) are evaluated numerically by Gaussian integration. This algorithm permits the exact integration of polynomials by simple summation of point values of the integrand. Mathematically, Gaussian integration is defined by

$$\int_{\tau=-1}^{\tau=1} f(\tau)\, d\tau = \sum_{KG=1}^{NP} G_{KG}\, f(\tau_{KG}) \qquad (100)$$

where:

$f(\tau)$ is the function to be evaluated from $\tau = -1$ to $\tau = +1$,
KG is the index number of the Gauss Point,
NP is the total number of Gauss points,
G_{KG} is a theoretically determined constant, and
τ_{KG} are the Gauss points.

Gaussian integration is well suited to two-dimensional groundwater modeling, and SUTRA was designed to satisfy its modest requirements. All finite elements can be transformed to the local coordinates, ξ and η, which vary from -1 to +1 (Figure 19). Because the weighting functions are either first- or second-order, only two Gauss points are needed per coordinate dimension , and all the constants are $G_{KG} = 1$.

SUTRA performs Gaussian integrations in three steps. First, the integral is converted to local coordinates. Second, the values of the integrand at the four Gauss points are calculated and summed. Third, the results are transformed back to global coordinates.

4. Matrix Form of Equations (76) and (97)

The finite difference form of the flow and solute/energy balance equations (Equations 76 and 97) can be solved simultaneously for the unknowns through the use of matrix algebra methods. This solution procedure is performed automatically by the SUTRA program, provided the input data is entered correctly.

First, the equations are placed in two groups, one for the unknown heads and one for the unknown concentrations or temperatures. Within each group, the equations are rewritten in identical, parallel form. All terms containing a variable (h_i or U_i) remain on the left side of the equal sign, and all known (constant) terms are moved to the right side.

The parallel equations are then converted to matrix form. A slightly simplified matrix equation of the flow balance is shown in Figure 23. Next, the matrix equations are streamlined as shown in Figure 24. This final system is solved using matrix algebra algorithms.

The matrix equations are solved for each time period. The input data are stored in arrays for efficient transfer to these matrices. During the first time period, the initial conditions are entered on the right side of the system; the boundary conditions on the left side and each constant parameter is entered on the appropriate side. The equations are solved for the unknown heads (h_i^1) and concentrations (U_i^1).

The matrix equations are then solved for the second time period. The values, h_i^1 and U_i^1, are now know quantities and are transferred to the right side of the system, replacing h_i^0 and U_i^0. Boundary conditions are updated, where necessary, and the matrix equations are solved again for the values of h_i^2 and U_i^2. This is repeated for all remaining time steps.

E. PROGRAM STRUCTURE AND SUBROUTINE DESCRIPTIONS

SUTRA was written in a modular, top-down format designed for code readability and ease of tracing the logic. Each major step of the program has been isolated in a subroutine. Most future revisions will involve only one or two subroutines. A logic flowchart, Figure 25, has been reproduced from the user's manual, to show the ordering of the subroutines. Table 5 is a brief description of the purposes of each subroutine. Using the chart and table together, one can follow the logic of the program.

$$\left(\frac{1}{\Delta t_{n+1}}\right)\begin{bmatrix} S_1V_1^{n+1} & 0 & 0\cdots 0 \\ 0 & S_2V_2^{n+1} & 0\cdots 0 \\ 0 & 0 & S_3V_3^{n+1} \quad 0 \\ \vdots & \vdots & \vdots\ddots\vdots \\ 0 & 0 & 0\cdots S_{NN}V_{NN}^{n+1} \end{bmatrix}\begin{Bmatrix} h_1^{n+1} \\ h_2^{n+1} \\ h_3^{n+1} \\ \vdots \\ h_{NN}^{n+1} \end{Bmatrix}$$

$$+\begin{bmatrix} I_{11}^{n+1} & I_{12}^{n+1} & I_{13}^{n+1} & I_{14}^{n+1} & \cdots & I_{1,NN}^{n+1} \\ I_{21}^{n+1} & I_{22}^{n+1} & I_{23}^{n+1} & \cdots & & \\ I_{31}^{n+1} & I_{32}^{n+1} & I_{33}^{n+1} & \cdots & & \\ I_{41}^{n+1} & \cdots & & & & \\ \vdots & & & & & \\ I_{NN,1}^{n+1} & \cdots & & & & I_{NN,NN}^{n+1} \end{bmatrix}\begin{Bmatrix} h_1^{n+1} \\ h_2^{n+1} \\ h_3^{n+1} \\ \vdots \\ h_{NN}^{n+1} \end{Bmatrix}$$

$$= \left(\frac{1}{\Delta t_{n+1}}\right)\begin{Bmatrix} S_1 & V_1^{n+1} & h_1^n \\ S_2 & V_2^{n+1} & h_2^n \\ S_3 & V_3^{n+1} & h_3^n \\ \vdots & & \\ S_{NN} & V_{NN}^{n+1} & h_{NN}^n \end{Bmatrix} + \begin{Bmatrix} Q_{IN_1} \\ Q_{IN_2} \\ Q_{IN_3} \\ \vdots \\ Q_{IN_{NN}} \end{Bmatrix} + \begin{Bmatrix} Q_1^* \\ Q_2^* \\ Q_3^* \\ \vdots \\ Q_{NN}^* \end{Bmatrix}$$

Figure 23. Simplified Balance Equations in Matrix Form.

$$
\begin{bmatrix}
\left(\frac{S_1 V_1^{n+1}}{\Delta t_{n+1}} + I_{11}^{n+1}\right) & I_{12}^{n+1} & I_{13}^{n+1} & \cdots & I_{1,NN}^{n+1} \\
I_{21}^{n+1} & \left(\frac{S_2 V_2^{n+1}}{\Delta t_{n+1}} + I_{22}^{n+1}\right) & I_{23}^{n+1} & \cdots & \vdots \\
I_{31}^{n+1} & I_{32}^{n+1} & \ddots & & \vdots \\
\vdots & \vdots & & \ddots & \vdots \\
I_{NN,1}^{n+1} & \cdots & \cdots & \cdots & \left(\frac{S_{NN} V_{NN}^{n+1}}{\Delta t_{n+1}} + I_{NN,NN}^{n+1}\right)
\end{bmatrix}
\begin{Bmatrix} h_1^{n+1} \\ h_2^{n+1} \\ h_3^{n+1} \\ \vdots \\ h_{NN}^{n+1} \end{Bmatrix}
$$

$$
= \begin{Bmatrix}
\frac{S_1 V_1^{n+1} h_1^n}{\Delta t_{n+1}} + Q_{IN_1} + Q_1^* \\
\frac{S_2 V_2^{n+1} h_2^n}{\Delta t_{n+1}} + Q_{IN_2} + Q_2^* \\
\vdots \\
\frac{S_{NN} V_{NN}^{n+1} h_{NN}^n}{\Delta t_{n+1}} + Q_{IN_{NN}} + Q_{NN}^*
\end{Bmatrix}
$$

Figure 24. Simplified Balance Equations in Streamlines Matrix Form.

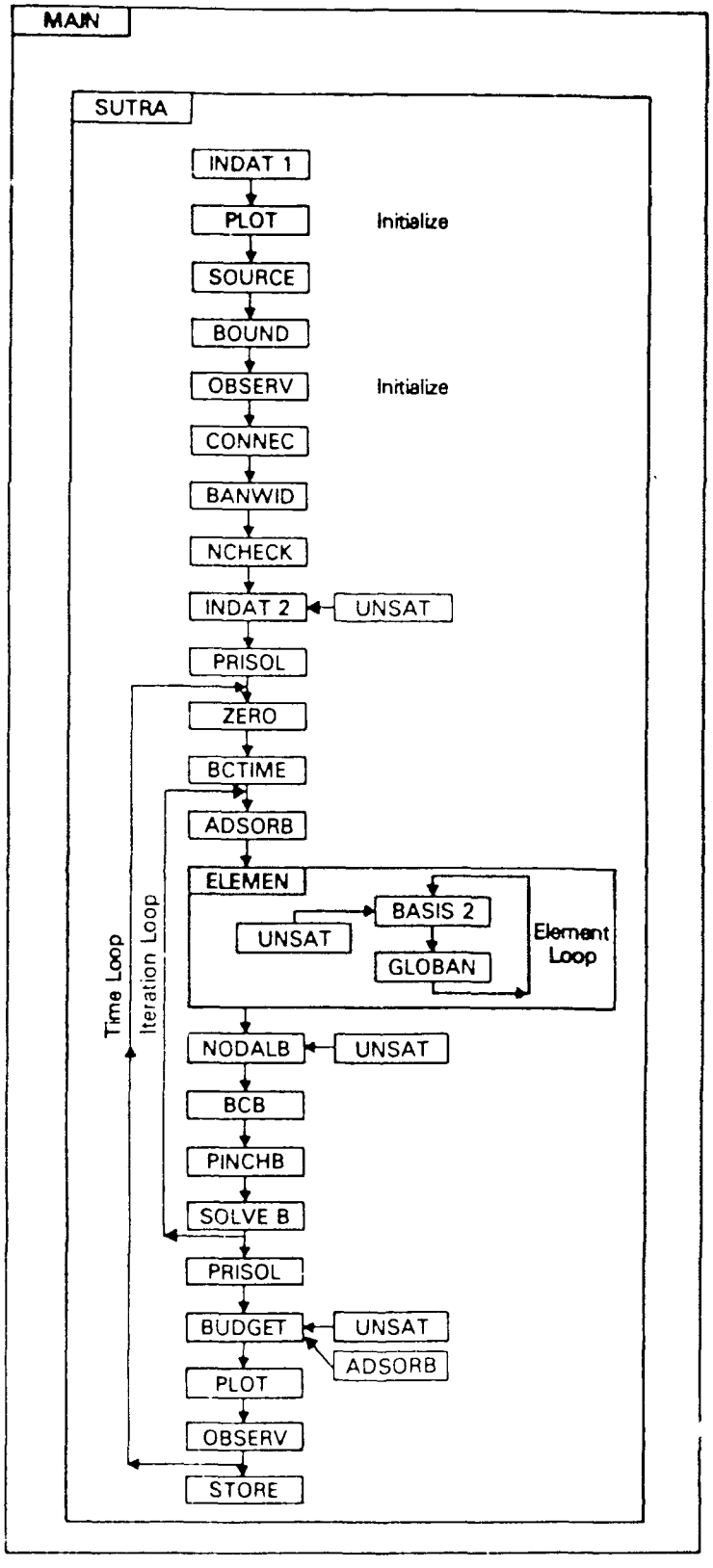

Figure 25. SUTRA Logic Flow.

TABLE 5. THE PURPOSES OF SUTRA SUBROUTINES.

Main Program:

- To determine whether the simulation will include energy transport, solute transport, or only groundwater flow.
- To dimension and allocate space for the main storage arrays.
- To divide the common storage arrays into their component arrays (set up pointers).
- To start and stop the simulation.

SUTRA:

- To act as primary control on SUTRA simulation, cycling both iterations and time steps.
- To sequence program operations by calling subroutines for input, output, and most program calculations.
- To carry out minor calculations.

INDAT1:

- To read simulation and mesh data from the Unit 5 data file, and print out this information.
- To (optionally) initialize some variables and carry out minor calculations.

PLOT:

- To provide maps on printer output paper of the finite-element mesh, pressure values at nodes, and U-values at nodes.

SOURCE:

- To read source node numbers and source values for fluid mass sources and boundary fluxes and for diffusive and productive U sources, as well as fluxes of U at boundaries.
- To check the data and to print information.
- To set up pointer arrays which track the source nodes for the simulation.

TABLE 5. THE PURPOSES OF SUTRA SUBROUTINES (CONTINUED).

BOUND:

- To read specified pressure node numbers and pressure values, to check the data, and print the information.
- To read specified concentration or temperature node numbers and values, to check the data, and to print information.
- To set up pointer arrays which track the specified p and U nodes for the simulation.

OBSERV:

- To save p and U values at chosen observation nodes as a function of the time.
- To report the observations after the simulation has been completed.

CONNEC:

- To read, output, and organize node incidence data.
- To read, output, and organize pinch-node incidence data.

BANWID:

- To calculate the band width of the mesh.
- To check the value specified by the user.

NCHECK:

- To check that pinch nodes are not assigned sources, nor have specified p or U.

INDAT2:

- To read initial conditions, EITHER:
  - cold start from Unit 55. (p, U)
  - warm start from Unit 66. (p_i, U_i, CSI_i, SW_i)

    $CS_i = C_{si}$; RCIT(i) = $\rho_o - \frac{\partial \rho}{\partial C}(C_i - C_o)$; $SW_i = S_{wi}$
- To initialize some arrays.

TABLE 5. THE PURPOSE OF SUTRA SUBROUTINES (CONTINUED).

PRISOL:

- To output the following to Unit 6:
  - Initial conditions
  - Pressure solutions
  - Saturation values
  - Concentration and temperature solutions
  - Steady-state pressure solution
  - Fluid velocities (magnitude and direction)

ZERO:

- To fill a real array with a constant value.

BCTIME: (user-programmed)

- To specify time-dependent pressure boundary conditions, and time-dependent temperatures or concentrations of the water flows that maintain these pressure boundary conditions.
- To specify time-dependent sources/sinks of solute mass or energy.

ADSORB:

- To calculate and supply values from adsorption isotherms to the simulation.

ELEMEN:

- To carry out all element-by-element calculations required in the matrix equations.
- To calculate element centroid velocities for output.

BASIS2:

- To calculate values of basis functions, weighting functions, their derivatives, Jacobians, and coefficients at a point in a quadrilateral element.

TABLE 5. THE PURPOSES OF SUTRA SUBROUTINES (CONCLUDED).

UNSAT: (user-programmed)

- To specify saturation as a function of pressure.
- To specify the derivative of saturation as a function of either pressure or saturation.
- To specify relative permeability as a function of either pressure or saturation.

GLOBAN:

- To assemble elementwise integrations into global matrix format.

NODALB:

- To calculate and assemble all terms specified by node (or by cell) in the matrix equation.

BCB:

- To implement specified pressure data conditions in the matrix equations.
- To implement specified temperature or concentration node conditions in the matrix equations.

PINCHB:

- To implement pinch-node conditions in both matrix equations.

SOLVEB:

- To solve a matrix equation with a nonsymmetric banded matrix.

BUDGET:

- To calculate and output a fluid mass budget on each time step with output.
- To calculate and output a solute mass or energy budget on each time step with output.

STORE:

- To store p and U results as well as other parameters on Unit 66 in a format ready for use as initial conditions (by INDAT2). This acts as a backup for restart in case a simulation is unexpectedly terminated before completion by a computer malfunction or programming problem.

SECTION V

CONTAMINATED GROUNDWATER SITE SELECTION

Real field data were desired to realistically check the capabilities and limitations of the three modeling programs. Originally, it was anticipated that IRP Phase II data could be used, but it was determined that a more detailed level of data was required for areal modeling programs.

After reviewing the operating manuals of the three groundwater/solute models and noting their input data requirements, available site data were collected and reviewed. As stated, the goal was to choose an IRP site with data suitable for "field tests" of the three models. Of the eight Air Force IRP sites reviewed, three had sufficient data (data beyond Phase II data) suitable for areal computerized modeling, and the Otis ANGB Sewage Treatment Plant plume was chosen as the most suitable for current purposes.

A. CHOICE CRITERIA APPLIED TO IRP REPORTS

Site selection was based on several modeling criteria. First, the necessary hydrologic site data should be available. Second, the aquifer should be suitable. It should be relatively homogeneous, unconsolidated, flat (no appreciable slopes), and relatively uniform. The aquifer should exhibit saturated flow conditions, and the water table should not change substantially with time. Third, there should be a readily modeled contaminant source which would be reasonably well defined, predictable over time, and affect an area convenient for modeling. Finally, the significant physical boundary conditions should be amenable to simulation by the computer models under evaluation.

The hydrogeologic data given in several of the IRP Phase I and II reports appeared generally favorable toward areal modeling. These Air Force bases are located in flat, unconsolidated, unconfined aquifers. In addition, each of these bases (five in number) had a number of contaminated sites from which to choose. However, many of the sites turned out to be unsuitable because heterogeneous deposits, such as braided river sediments, were present.

In these reports, a pattern of gathering IRP Phase II field data was noted. Field investigators located the contamination sites, then gathered relevant data from previous field studies. This included well drilling cores, from which geohydrology and water table levels were determined. From these data, the direction of near surface groundwater flow was determined, as well as possible plume migration. Then, the investigators drilled four monitoring wells, one up gradient and three down gradient of each selected contamination site. These wells yielded more hydrogeologic, water table, and contamination data.

The general suitability of Phase II IRP data for groundwater modeling can be explained with reference to Figures 26 and 27. The three downgradient wells in Figure 26 can be considered to fall on a straight line, or on the radius of a circle. Either way, the pattern is considered one dimensional. Data from these wells can identify the presence of a contaminant plume. However, to map a two-dimensional plume and verify modeling results, data must

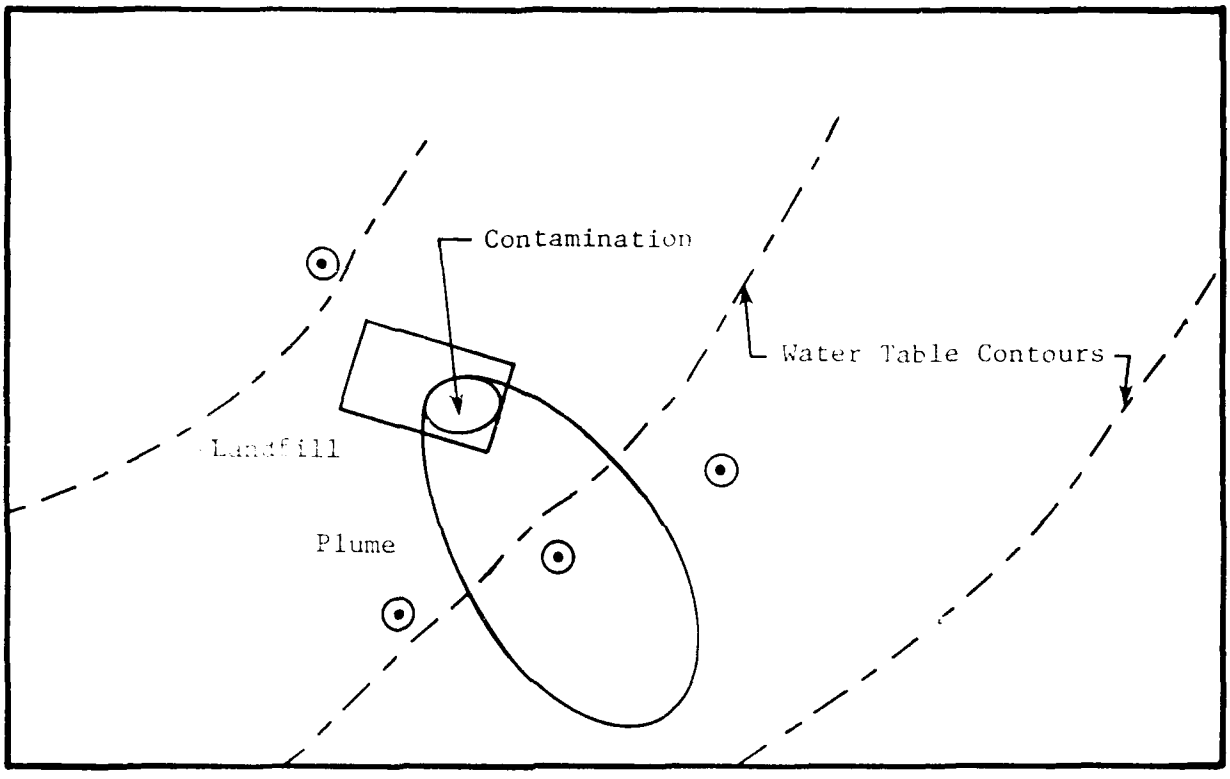

Figure 26. Typical IRP Phase II Well Field.

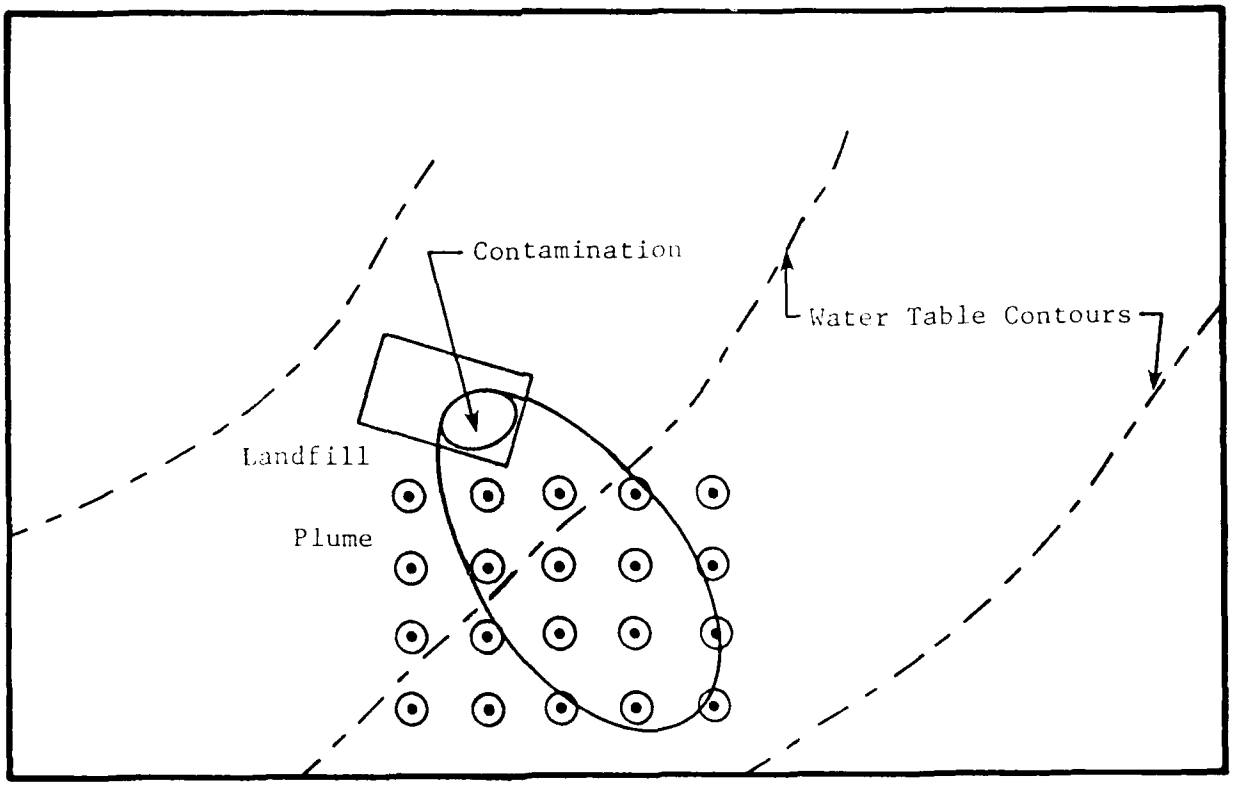

Figure 27. A More Ideal Well Field for Plume Modeling.

be taken with a two-dimensional well field. Figure 27 shows a more ideal well field, a two-dimensional grid of wells.

Only three Air Force installations had sufficient two-dimensional well field data: Air Force Plant 44, Wurtsmith AFB, and Otis ANGB.

B. ANALYSIS OF THE THREE AIR FORCE SITES

1. Plant 44 Data at Tucson, Arizona

The Plant 44 data (References 2, 9, 10) were initially studied in this project. The aquifer was reasonably level, unconsolidated, and had saturated soil conditions. Because local land use was significantly nonuniform, full physical property maps had been prepared. In addition, the site had been extensively investigated and modeled geohydrologically by Hargis & Montgomery using the USGS-2D model (Reference 2).

Certain drawbacks of this site were noted:

- The contaminant source term is not well defined, and varies with time. This would introduce another layer of uncertainty into the simulation tests.
- The aquifer covers a large area, and some of the parameters vary substantially with position in the aquifer. This would increase the complexity of the modeling effort.
- The water table varies significantly over time. This would also complicate the modeling effort. Hargis and Montgomery used four separate time periods to simulate the plume's migration.

The effort required to model a complicated site like Air Force Plant 44 would have gone well beyond the intended scope of our project.

2. Wurtsmith AFB Data

The next site studied in the project was Wurtsmith AFB (References 1, 11, 12, 13). This site has several attractive features:

- The aquifer is a level, homogeneous, unconsolidated, and unconfined.
- The area to be modeled is smaller and simpler than Plant 44.
- There are no leaky artesian aquifer boundaries. This would simplify the simulation.
- Due to plume containment measures, which changed with time, and for which data had been recorded, one could independently calibrate and predict simulation runs.

- The particular spill has been modeled by USGS hydrologists (see Reference 1), using USGS modeling programs based on the algorithm of Trescott, Pinder, and Larson (see Reference 14).

There are also some serious drawbacks:

- Flow rates of a number of wells varied with time. This would complicate the modeling effort.

- The size and time-history of the contaminant spill are not well-known.

- The saturated thickness of the aquifer changes with time and position, due to well-pumping. Further, the effects of the pumping wells are magnified by the relatively thin saturated thickness.

- Well field data were not available in a timely manner.

Because of these problems for the project, the Otis ANGB sewage plume was chosen for the project.

3. Otis ANGB Data

Otis ANGB occupies the southern end of the Massachusetts Military Reservation, which is located on western Cape Cod, Massachusetts. Two groundwater pollutant plumes run south from just within the southern boundary of the base. The smaller plume contains TCE and its breakdown products (Figure 28). The size, location, and time-history of its source are not well known.

The larger plume, the 'sewage" plume, occupies much of the same space as the TCE plume, but has a greater extent. Its source is the Otis ANGB sewage treatment plant. The secondary sewage effluent from the plant is sprayed over sand beds for its final treatment. As this effluent percolates down into the groundwater, the remaining chemically digestible contaminants are removed, but some inorganics remain. This latter plume was chosen for the current study because it has been extensively studied, has a relatively well-defined source term, and has already been numerically modeled. A number of inorganic contaminants are present in the sewage plume, including boron, nitrate, phosphate, detergent, sodium and chloride. Boron was chosen for the current study because it is conservative (not adsorbed on the soil particles), stable, and effectively absent from clean, natural groundwater (Reference 16).

A number of reports on this plume were reviewed, including: IRP Reports (References 15, 16), USGS Open File Reports (References 17, 18), a contractor report (Reference 19) and a number of other reports containing general hydrologic information on Cape Cod.

For 40 years, the sewage effluent and its residual contaminants have formed a plume moving generally south with the regional groundwater. The USGS has carefully studied this plume for several years. Pertinent data collected by this group are reproduced in the following forms:

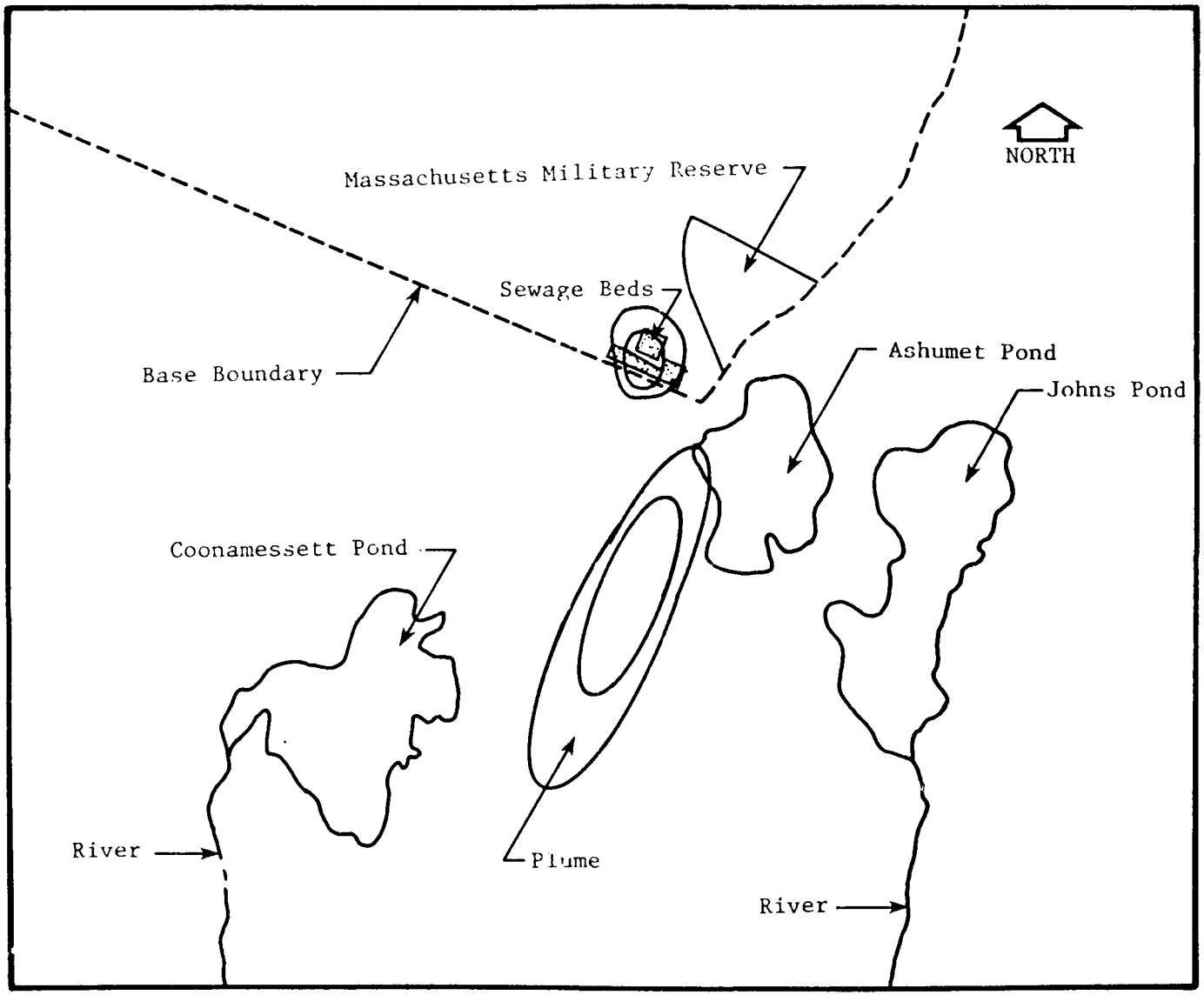

Figure 28. Map of Chlorinated Ethenes in Otis ANGB Groundwater (Reference 15).

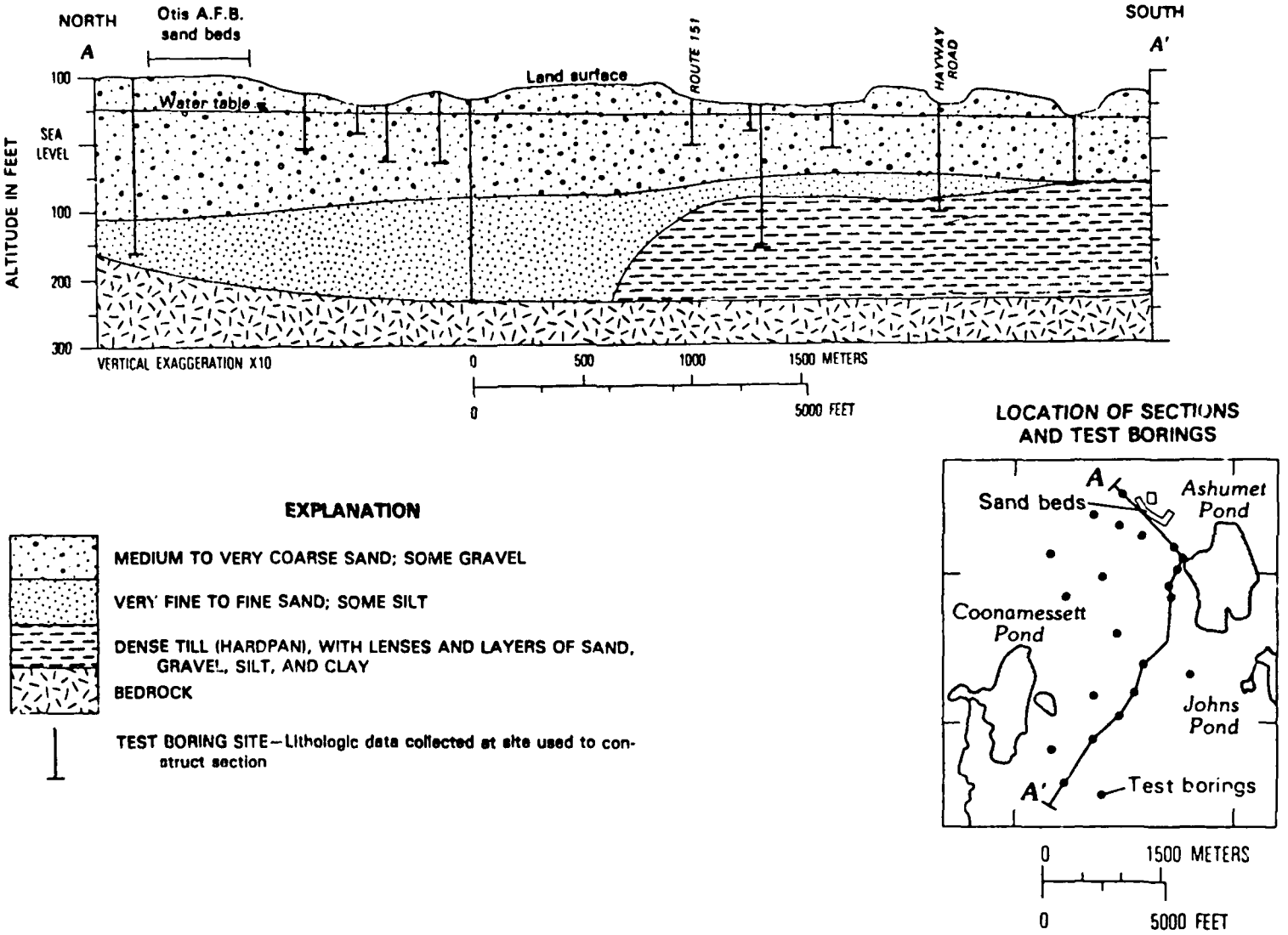

Figure 29. Geologic Section Showing Hydrogeologic Units in the Study Area (Reference 18).

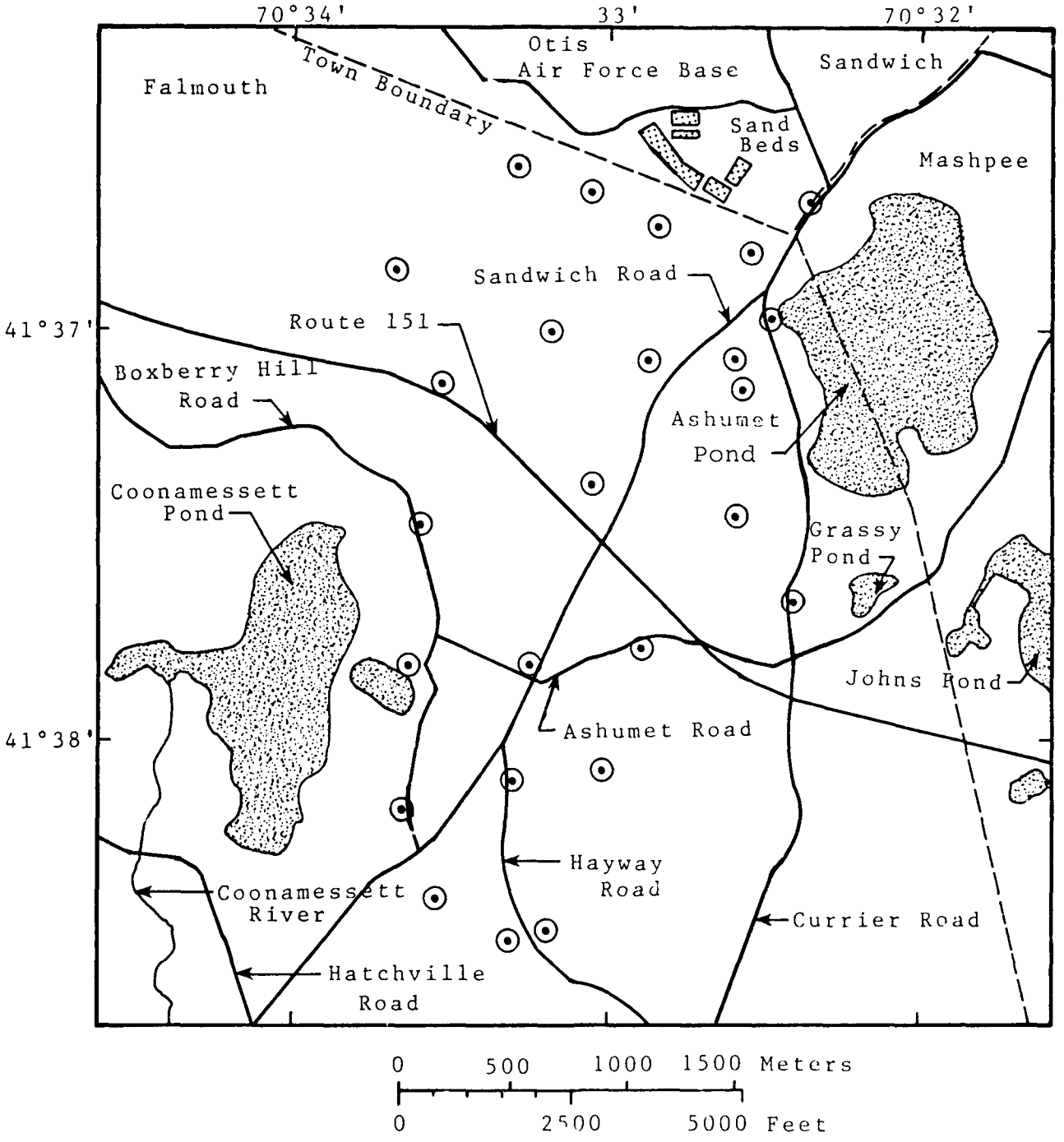

Figure 30. Map of USGS Well Field Near Ashumet and Grassy Ponds (Reference 18).

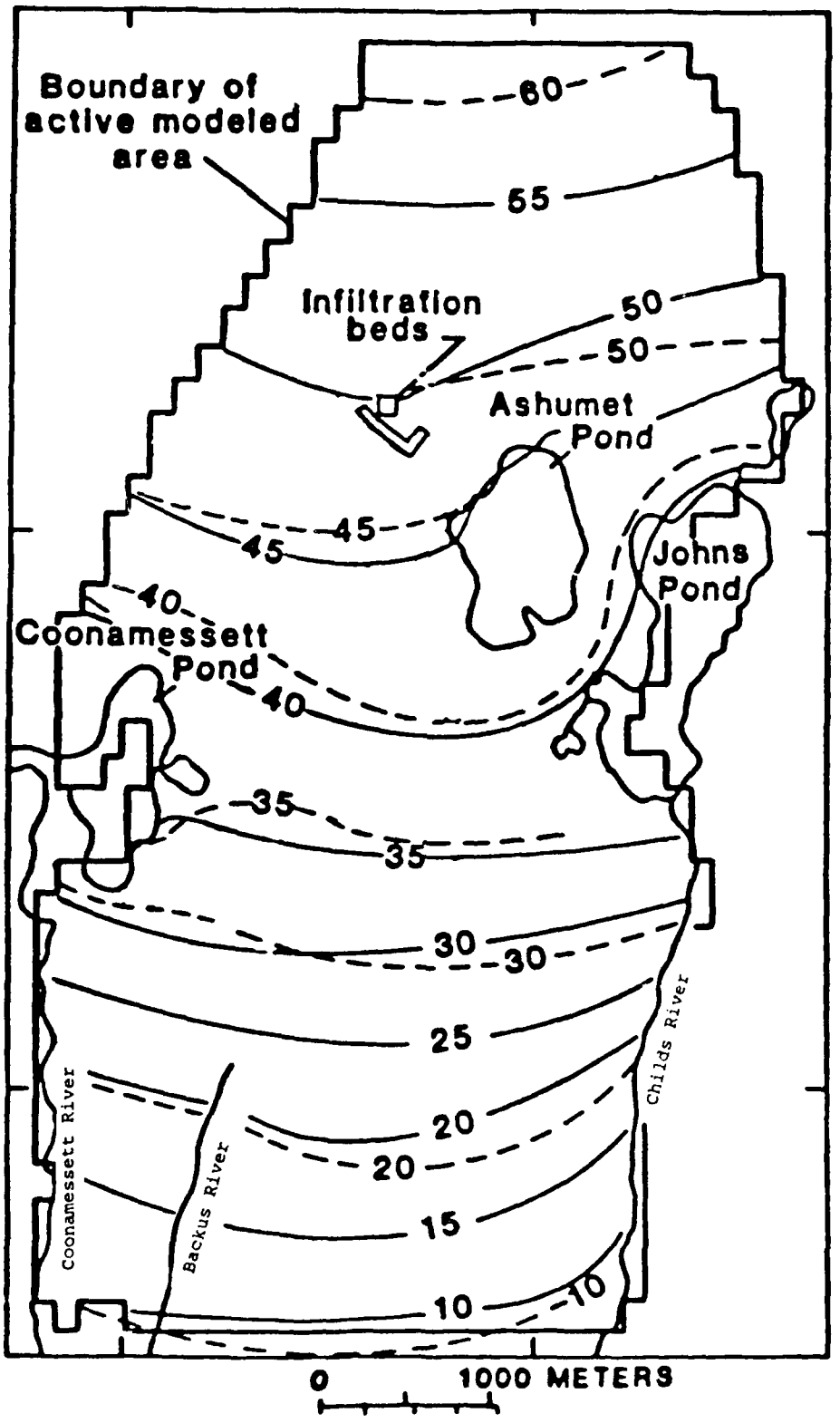

Figure 31. Water Table Contours in the Modeled Areas at Otis (Reference 18).

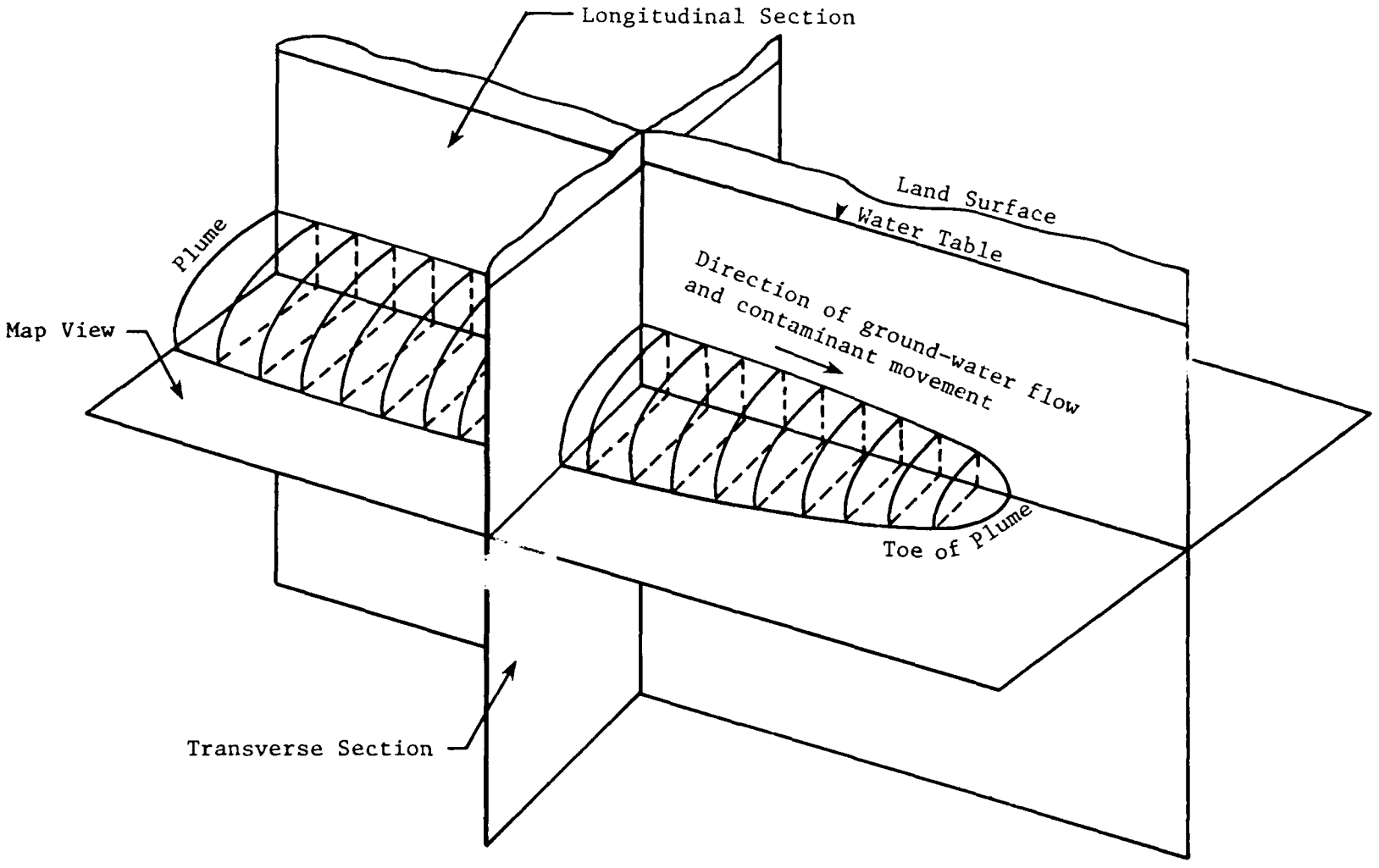

Figure 32. Three-Dimensional Diagram Showing Vertical Stratification of the Otis Sewage Plume (Reference 18).

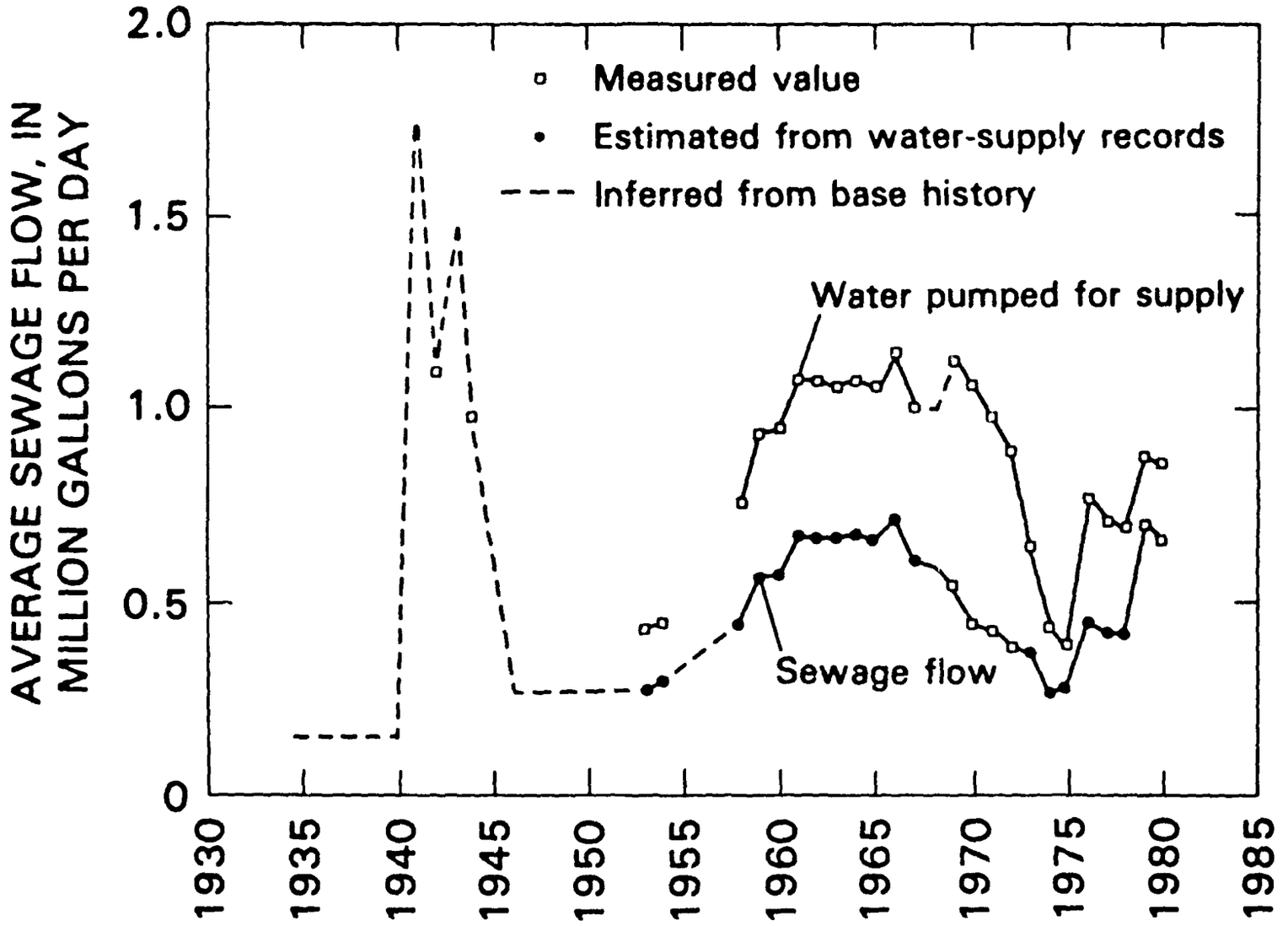

Figure 33. Volume of Sewage Treated at the Otis Air Force Base Treatment Plant from 1936 Through 1980 (Reference 18).

SECTION VI

SIMULATION RESULTS USING THE USGS-2D MODEL

A. INTRODUCTION

Modeling efforts using the USGS-2D program involved four major phases. Since the source program had previously been installed on the CYBER system, phase one was Preparation. In this phase, the aquifer discretization or cell size was chosen, the input data file was prepared, and the source code arrays were appropriately redimensioned. The second phase consisted of Implementation where standard familiarization/test cases were run and problems were corrected as needed, to permit complete successful runs of the program. For example, one fatal data format error was particularly troublesome until corrected. In phase three, Calibration, several minor typographical errors were corrected. Then, efforts were centered on Ashumet Pond at Otis ANGB site. The pond's boundary conditions and its material balance were checked. Finally, in the Sensitivity Study Phase, thirteen parameters were tested. Plume maps are shown in this report for all parameters which exhibit noticeable sensitivity effects.

B. PREPARATION AND IMPLEMENTATION

1. Preparation Phase

The first step in modeling is preparation of the input data file. LeBlanc's discretization of the aquifer was initially used (Figure 34), along with his published input parameters (Reference 18). He had used these values successfully in modeling the Otis plume with the USGS-2D program. While not all of the required input were published, those data that were published are listed in Table 6. Values assumed for the remaining parameters are listed in Table 7.

2. Implementation Phase

Initially, the familiarization/test problems in the back of the user's manual were considered (Reference 3). The source program had already been installed and run on the CYBER system. The CYBER system debugging option (Post Mortem Dump) was used to update two minor input data format changes. All three test problems then ran successfully with the updated system.

Then the input data file for Otis was prepared. An annotated input data file template is shown in Appendix D. For reference, the input data files on this system are named WHKBOT i, where i is a letter from A to Z. The dimensions of the aquifer map arrays (in COMMON storage) were increased to accommodate the Otis grid.

Initial Otis simulation runs blew up due to execution time errors, which were difficult to diagnose, even with full dump printouts from several debugging runs. However, the problem turned out to be an inadvertent violation of an input data format requirement. The user must explicitly specify a zero thickness for all impermeable cells, including the outermost rows and columns. Unlike the transmissivity data map, the program does not

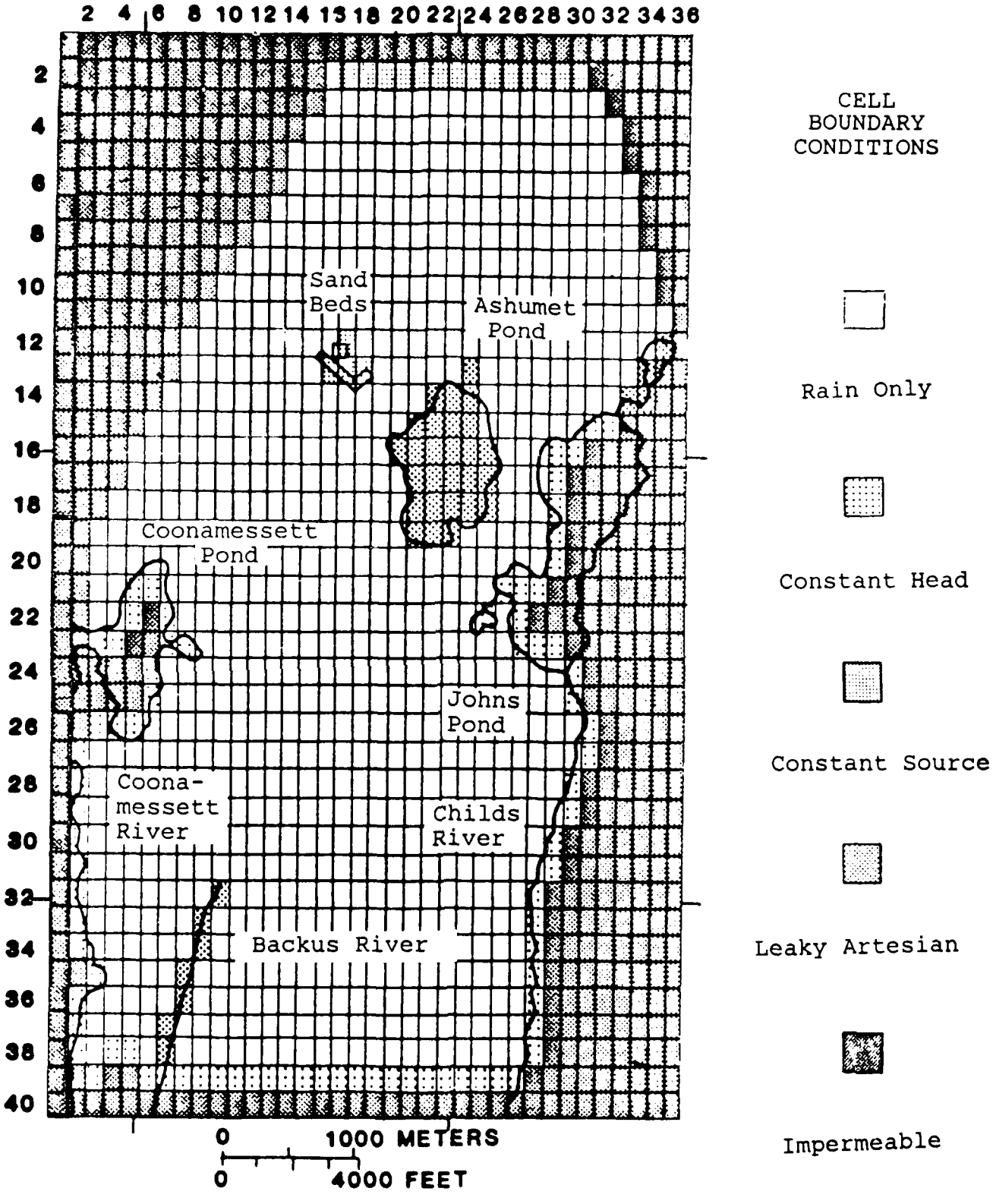

Figure 34. USGS-2D Grid for Otis Sewage Plume (Reference 18).

TABLE 6. LEBLANC'S PUBLISHED INPUT PARAMETERS (REFERENCE 17).

Parameter	Description	Value
PINT	Total simulation time period (years)	40.
NX	Spatial discretization (No. of columns)[a]	36
NY	Spatial discretization (No. of rows)[a]	40
XDEL	Cell width (feet)	750.
YDEL	Cell length (feet)	1500.
POROS	Porosity, (vol. fraction)	0.35
BETA	Dispersivity, longitudinal (feet)	40. - 100.
BETA*DLTRAT	Dispersivity, transverse (feet)	13. - 33.
NCODES	(No. of different types of boundary conditions)	6
PERM(I,J)	Hydraulic conductivity, assumed isotropic (ft/day)	187.[b]
NPMP	Number of pumps	0
THCK(I,J)	Cell thickness (feet)	c
WT(I,J)[d]	Pond levels (feet above mean sea level)	
	Ashumet:	44.7
	Johns:	38.7
	Coonamessett:	33.7

a Includes impermeable boundary cells.

b LeBlanc said that the average of several field tests was PERM = 170 ft/day, but that his computer modeling calibration supported PERM = 187 ft/day.

c A thickness trace plot was published (Figure 29) but it was not a complete aquifer thickness map.

d WT(I,J) values are initial conditions, except in cells where leakance is nonzero. In leaky artesian cells, WT(I,J) is a boundary condition, as well as the ponds.

TABLE 6. LEBLANC'S PUBLISHED INPUT PARAMETERS (CONCLUDED).

Parameter	Description	Value
VPRM(I,J)[e]	LeBlanc's values for Ashumet Pond Leakance Coefficients (ft/sec):	e
	At pond edges	1.0E-4[f]
	At pond center	2.0E-6
RECH(I,J)	Net rainfall/recharge rate (in/yr) for:	g
	Average annual rainfall:	46.7
	Average annual evapotranspiration + pumpout	25.7
	Runoff assumed negligible due to sandy soil	0.0
	Net average recharge:	
	(in/yr)	21.0
	(ft/sec)	5.46E-8[h]
RECH()	40-Year average sewage source term[i] (ft^3/sec @ 500 ppb)	1.8
RECH()	Average source term along northern boundary of modeled area, flow from upgradient (ft^3/sec)[j]	2.3
WT(I,J)	Boundary values and initial water table value map[j]	

e Referring to the values entered in Data Set No. 7 in Appendix C.

f Effectively a constant-head cell (≥ 1.0E-5).

g Entered in Data Set No. 5 in Appendix C.

h Entered in Data Set No. 7 in Appendix C.

i This rate has varied substantially over the years, along with the number of troops stationed at Otis Figure 33.

j Correct values for the initial conditions are unimportant.

TABLE 7. UNPUBLISHED INPUT PARAMETERS.

Parameter	Description	Value
NTIM	Number of time periods in groundwater head simulation for steady-state cases	1
TOL	Use the tightest standard convergence[a] tolerance for the head solver algorithm	0.0001'
S	Storativity for steady-state flow cases	0.0[b]
TIMX	Time Increment Multiplier	0.0[b]
TINIT	Initial time increment (sec)	0.0[b]
NPMP	Number of pumps with appreciable flow rates	0
CELDIS	Maximum particle travel distance before velocity reinterpolation (fraction of cell length or width)	0.2
NUMOBS	Number of observation wells	0[c]
CONC(i,j)	Initial solute concentration in cell(ppb)[d] (no solute present initially)	0.0

a The largest change in calculated head of any cell over the current iteration.

b That is, these parameters are not used in steady-state flow cases.

c Optional, 0 to 5.

d Normally ppm. Assumed to be ppb in this project.

zero the cell thicknesses at the edge of the thickness map. This requirement was not explicitly stated in the input data instruction section of Reference 3.

C. CALIBRATION

First, typographical errors were found and corrected. Because the input data file was several pages long; this required several runs. Once this was done, the simulated hydraulic head map and plume map agreed reasonably well with LeBlanc's results. However, for general applications of this model, fewer input parameters will be predetermined and much more effort will be required in adjusting unknown input parameters values.

1. Groundwater Head Distribution

Solution for groundwater heads is straightforward. The simulated head map for the Otis plume is shown in Figure 35. Comparing this map to LeBlanc's simulation and the corresponding field data in Figure 35 indicates that the two maps are quite similar.

Both simulated maps show that the head values north of the sand beds are up to 3 feet low at the northern boundary. Neither study explains this satisfactorily. Our attempt to decrease saturated thickness north of the sand beds failed to noticeably improve the fit. Fortunately, that area is relatively unimportant to the overall situation, and the fit is adequate elsewhere.

2. Solute Transport

Next, the solute material balance was studied. The program keeps running totals of the solute mass entering and leaving the aquifer. In the Otis case, solute enters only through the sewage treatment beds and leaves only through sinks which are specified as leakance or constant head cells. Over the 40-year simulation, approximately 40 percent of the solute entering the system leaves through these sinks. The computational domain's four main boundaries (N,E,S,W) are impermeable. There are sinks at the ponds and rivers. Of these sinks, solute reaches only Ashumet Pond in significant quantities. Therefore, approximately 40 percent of the solute enters Ashumet Pond.

There is a reasonable physical mechanism to explain these solute losses. Because the ground slopes to the south, and Ashumet Pond has no sources or sinks other than groundwater, the northern half of the Ashumet Pond cells functions as sink cells and the southern half function as source cells. Thus, groundwater is taking the path of least resistance through the pond, and bypasses several cells in the process. Vertical flows into the pond are illustrated in Figure 36 and horizontal flows are illustrated in LeBlanc's plume maps, (see Reference 18), where the groundwater flowing from the sewage beds is first drawn in the direction of the Ashumet Pond sink cells.

However, there is an apparent discrepancy in the fate of the solute that enters Ashumet Pond. The USGS-2D program has no provisions suitable

Figure 35. Simulated Water Table Contours Using USGS-2D Program and Otis ANGB Data.

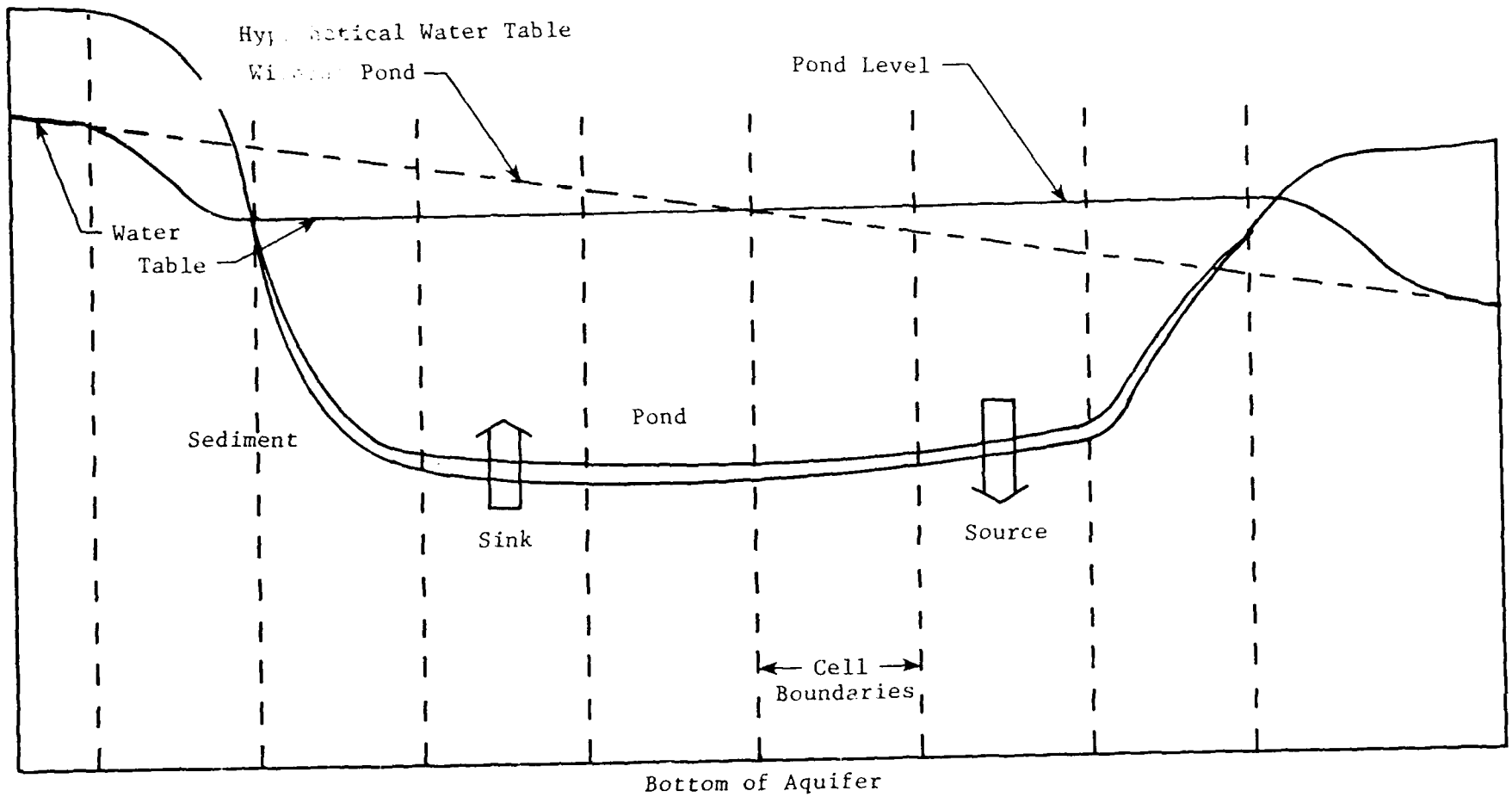

Figure 36. Ashumet Pond Level, Sources, and Sinks.

for reinjecting the solute from the pond back into the ground. LeBlanc's report (Reference 18) implies that in his modeling, solute entering Ashumet Pond remains there. In spite of the simulated results, the field data does not indicate a major buildup of solute in the pond. So, one would expect LeBlanc's calculated concentration plume to be smaller than the field-measured plume, reflecting the unaccountable solute. But, LeBlanc's calculated concentration plumes do not appear smaller.

As implied, the USGS-2D model has incomplete provisions for the transport of solute through the bottom of a pond or river. The model accounts properly for solute in the groundwater leaking into the pond. However, for contaminated pondwater reentering the ground, source concentration values must be entered, cell by cell, in Data Set 7 (see Appendix C). Because solute concentrations in the pond vary with time, and are unknown ahead of time, the source concentration values entered into Data Set 7 are time dependent. But, the program is written and formatted to accept only constant numerical values, zero in this case. Thus, it appears that any solute entering Ashumet Pond is lost in the simulation.

It appears unlikely that LeBlanc modified the program to properly reinject pondwater solute. Adapting the program to calculate the solute concentration in the pond over time, and to accept variables for input concentrations would be an appreciable program modification. LeBlanc (Reference 18) described his modeling efforts in considerable detail, and mentioned no program modifications for solute recharge at Ashumet Pond.

Field data are not consistent with a major accumulation of solute in Ashumet Pond. For the pond to accumulate 40 percent of the total solute, its solute concentration would have to build up throughout the pond. LeBlanc's published concentrations contours do not show this. And, more important, solute would be reentering the groundwater along the entire southern half of Ashumet Pond. If so, one would expect a broader plume and an appreciable solute concentration in the groundwater from the well nearest Grassy Pond, due south of Ashumet Pond (see Figure 30). Field data show that solute concentrations are rather low in this area.

Two inferences may be drawn from this:

a. The model calculations do not account for a substantial portion of the solute that is probably present in the plume.

b. Since the calculated plume contours still match the field data pretty well, either:

   (1) the plume maps are relatively insensitive to the total amount of solute present; or

   (2) other input parameters were inadvertently distorted, thus masking the error at Ashumet Pond; or

   (3) vertical stratification effects are masking leakance effects at Ashumet Pond;

(4) much of the solute in Ashumet Pond chemically precipitates, mixes with the pond sediment, and thus is not present in either the plume or the pondwater.

Groundwater flow behavior also helps explain the shape of the plume. First, when water containing significant solute concentrations leaks into Ashumet Pond, it appears to flow due south, remaining in the western portion of the pond. Second, the calculations indicate that as contaminated water is drawn progressively under Ashumet Pond, this water progressively leaks upward into the pond, and contaminated water remaining in the ground mixes with and is diluted by more clean groundwater from elsewhere. This would explain the progressive drop in solute concentration as one moves away from the northwest corner of the pond.

Third, the flow behavior explains the failure of the plume to move further to the east. South of Ashumet Pond, the plume moves in a SSW direction as in Figure 37, the base case plume map. In a sensitivity study run where the bottom of the pond was assumed impermeable, the plume spread southeastward from the sand beds until it reached Johns Pond, and then spread due south between the Childs and Backas Rivers (Figure 38).

USGS-2D simulations revealed limitations in accuracy and precision in both the input and output. If several runs are made with exactly the same input parameters, the outputs will always be exactly the same (any errors will be identical). However, this study did not check to see if small changes in inputs (ΔI) result in small, smooth changes in output (ΔO) (Figure 39A), or whether there is superimposed noise due to discretization effects (Figure 39B).

D. SENSITIVITY

Thirty-six simulation runs were made to check the importance of variations in 13 input parameters. These runs are listed in Table 8. Two base case plume maps are included. One is given in Figure 37, and the other is that used by LeBlanc (Figure 40). A copy of the base case input data file is found in Appendix D.

1. Cell Thickness

LeBlanc's cell thickness data, THCK (I,J), were not available, so Figure 29 was used to estimate this parameter. These estimates probably have an uncertainty of 10 to 15 percent. A constant thickness value was assumed in each E-W row.

The thickness of the northernmost few rows of cells was reduced to try to get the groundwater head profile closer to the measured field values. However, the reduced thickness did not appreciably change the head profile or the plume map, compare Figures 31 with 35, and Figures 40 with 41. LeBlanc, too, had difficulties with the water table heads at this end of the aquifer (Reference 18).

2. Hydraulic Conductivity

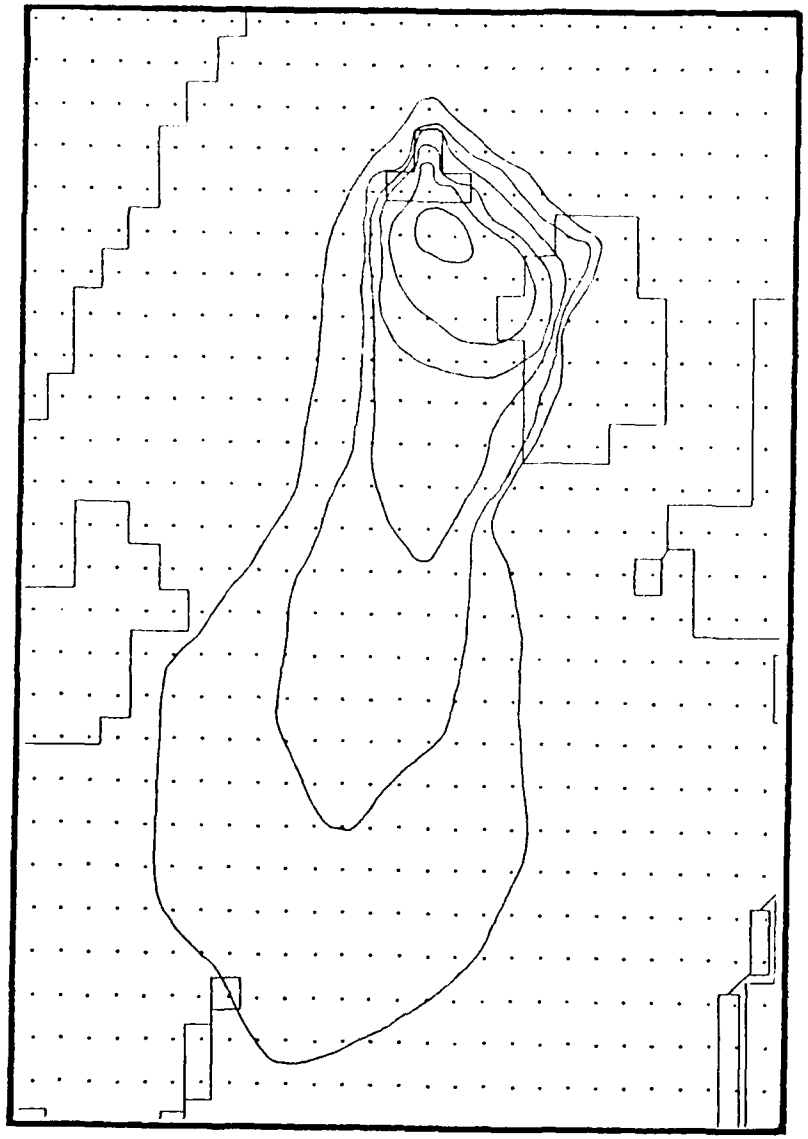

Figure 37. USGS-2D Base Case Plume Map for Otis ANGB.

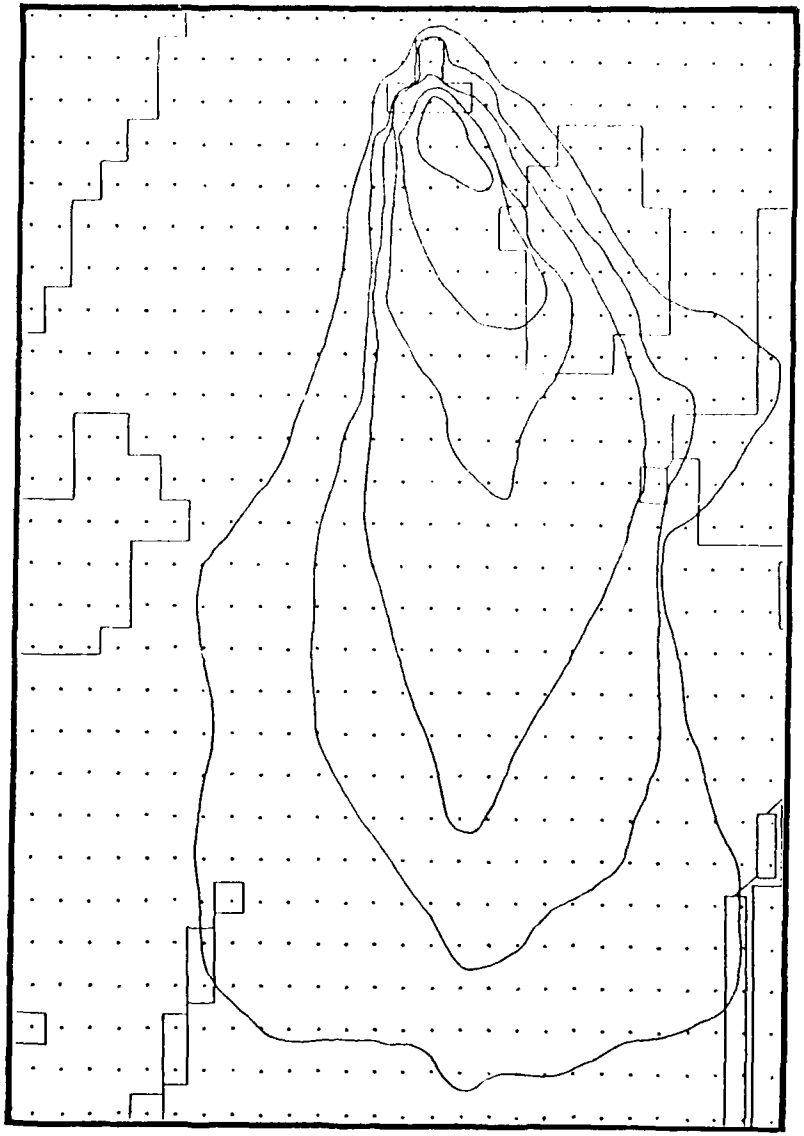

Figure 38. USGS-2D/Otis Plume Concentration Map with Ashumet Pond Leakance Coefficients Reduced 97 Percent.

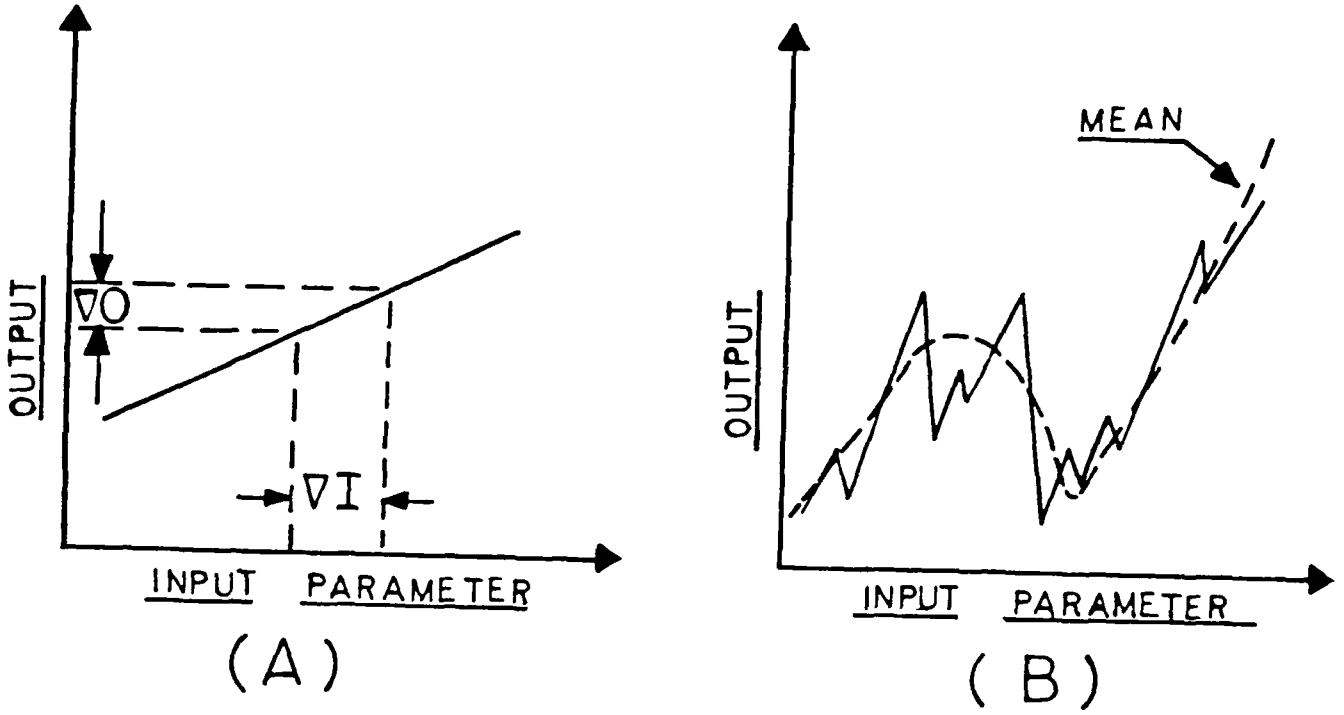

Figure 39. Considerations Not Explicitly Considered in this Study: (A) Small Input Changes Produce Small Output Changes, and (B) Discretization Effects Produce a Random Output Component.

TABLE 8. USGS-2D SENSITIVITY RUNS.

Run Notation WHKBOT(i) Where (i) Equals	Parameter Notation and Parametric Values	Parameter Names
A	max THCK ≈ 154 ft.	Maximum saturated thickness
B	max THCK ≈ 142 ft.	Maximum saturated thickness
C	max THCK ≈ 136 ft.	Maximum saturated thickness
D	K = 214 ft/day	Hydraulic Conductivity
E	K = 194 ft/day	Base Case, Hydraulic Conductivity
F	K = 178 ft/day	Hydraulic Conductivity
G	RECH = 6.27D-8 ft/sec[1]	Rainfall Recharge Rate
H	RECH = 4.18D-8 ft/sec[1]	Rainfall Recharge Rate
I	K = 234 ft/day	Hydraulic Conductivity
J	NPTPND = 9	Initial Particles/Cell
K	RECH = 5.23D-7 ft/sec	Rainfall Recharge Rate
L	BETA = 0.01 ft	Longitudinal Dispersivity
M	BETA = 100 ft	Longitudinal Dispersivity
N	CNRECH = 600 ppb	Boron Concentration[2]
O	CNRECH = 400 ppb	Boron Concentration[2]
P	RECH = 6.36 D-7	Sewage Flux @ Beds
Q	RECH = 4.36 D-7	Sewage Flux @ Beds
S	NPTPND = 8	Initial Particles/Cell
T	NPTPND = 4	Initial Particles/Cell
U	RECH[3] = 1.2D-4	Ashumet Pond Edge Leakance Coefficient
V	RECH = 0.8D-4	Ashumet Pond Edge Leakance Coefficient
W	RECH = 1.0D-7	Ashumet Pond Edge Leakance Coefficient
X	RECH = 1.0D-5	Ashumet Pond Edge Leakance Coefficient
Y	----------	Tilt East[4]
Z	----------	Tilt West[4]
A'	CELDIS[5] = 0.75	
B'	CELDIS = 1.00	
C'	CELDIS = 0.25	
F'	ANFCTR = 1.20	K_{yy} / K_{xx}
G'	ANFCTR = 0.80	K_{yy} / K_{xx}
J'	----------	Base Case[6]
K'	----------	Base Case[6]
L'	DLTRAT = 0.50	Transverse Dispersivity = 20 ft
M'	DLTRAT = 0.10	Transverse Dispersivity = 4 ft
N'	NPTPND = 4	Initial Particles/Cell

1 All permeable cells except ponds.

2 Rainwater + Sewage Basis.

3 Entered as FCTR1 in Data Set 7.

4 Slightly raised Coonamessett Pond level and slightly lowered Johns Pond level.

5 The distance, expressed as a fraction of cell length (or width) that a particle can travel before its velocity is recalculated.

6 Repeatability tests for base case.

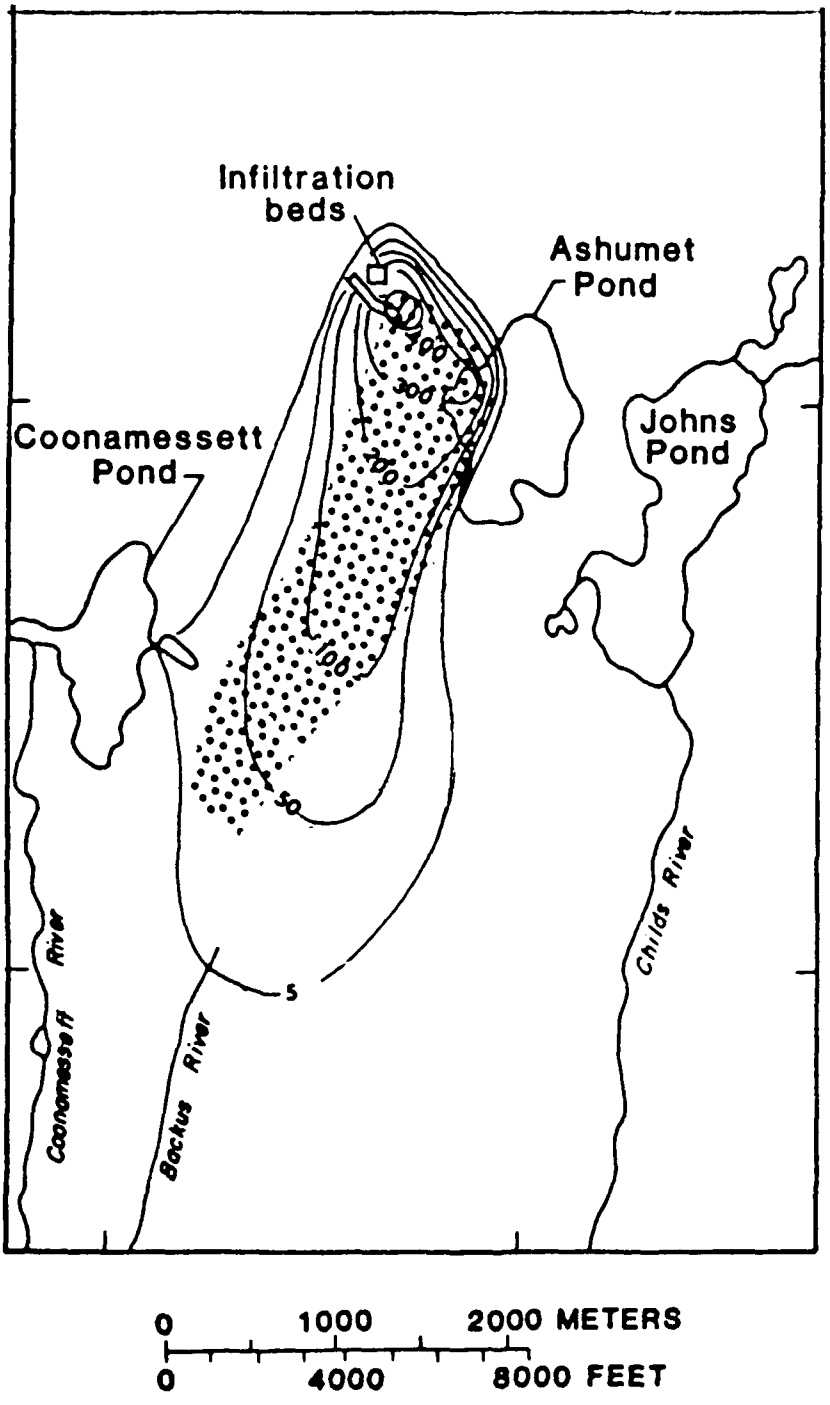

Figure 40. LeBlanc's Simulated and Measured Plumes (Reference 18).

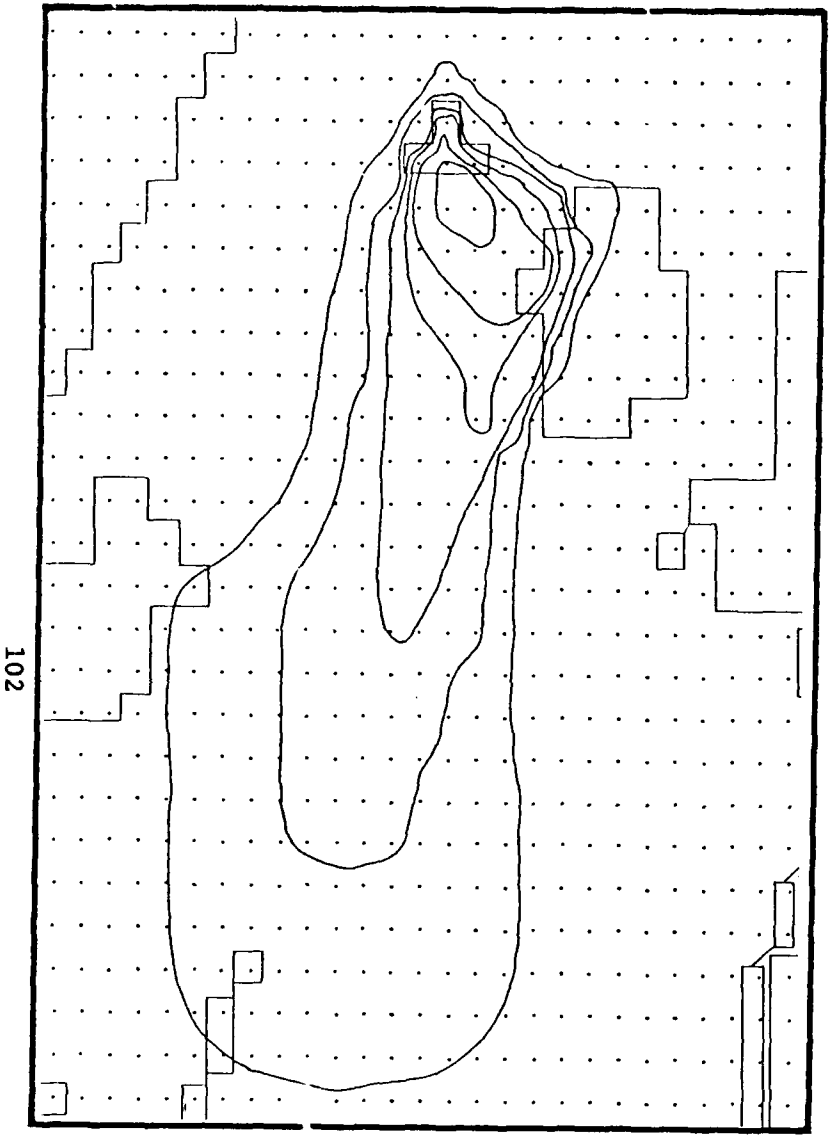

Figure 41. USGS-2D/Otis Plume Concentration Map for K = 214 ft/day.

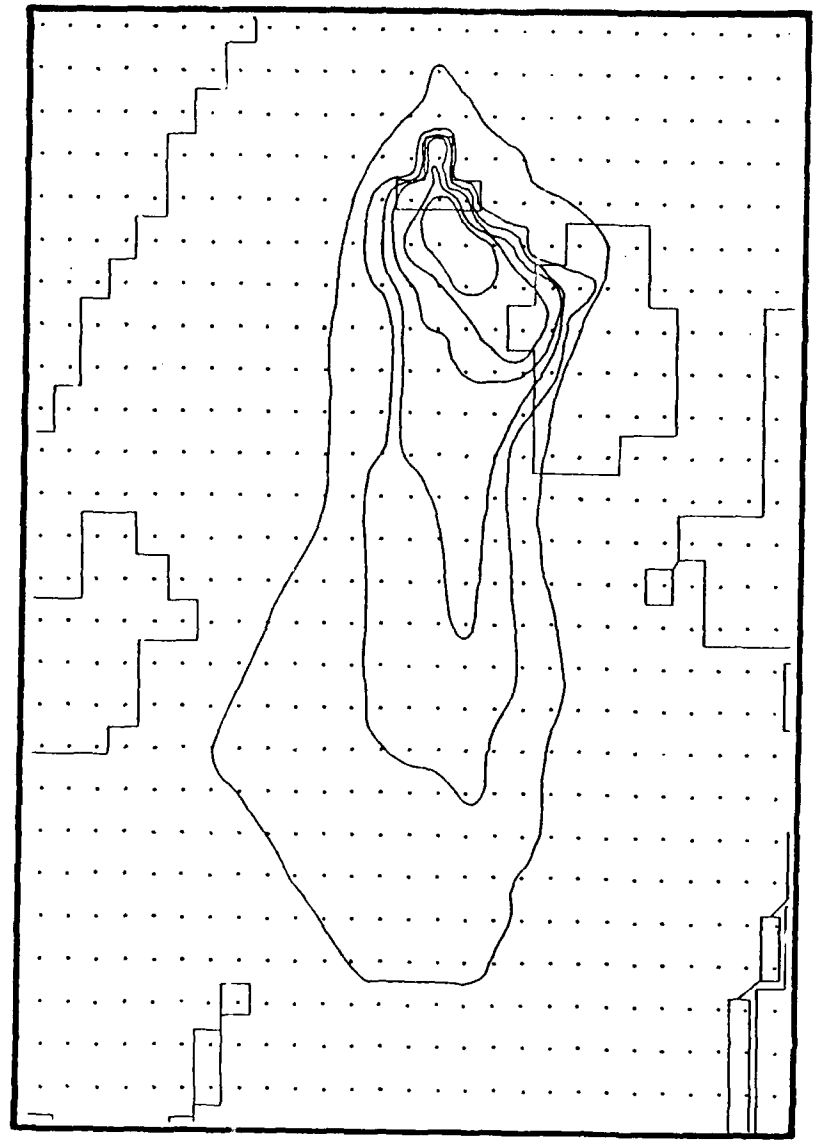

Figure 42. USGS-2D/Otis Plume Concentration Map for K = 178 ft/day.

The hydraulic conductivity, TMRX (I,J,1)/THCK(I,J), of the aquifer was varied by ±20 percent. There is at least that much uncertainty in this parameter because: (a) field test values are somewhat uncertain, even when available; (b) hydraulic conductivity can vary within an aquifer, and a test result may be valid only where measured; and (c) when test results are unavailable, estimation formulas must be used, and these estimates are even more uncertain than test values.

Hydraulic conductivity values must often be adjusted empirically during modeling for the calculated plume map to fit the field-measured concentration data. LeBlanc adjusted his hydraulic conductivity value from the field test value of 170 ft/day to 187 ft/day, based on modeling results. Our study used 194 ft/day as the base case value.

As hydraulic conductivity was increased, the simulated plume expanded accordingly. The plume changed visibly in length, but usually not drastically. The width of the plume, however, changed considerably more, compare Figures 41 and 42.

3. Solute Tracer Particles

The number of solute tracer particles, NPTPND, was varied by changing the number of particles per cell. At NPTPND = 9, the CYBER system's core capacity per user was at 99 percent of its limit. The resolution was slightly better than at NPTPND = 5, but there were no important changes in the simulated plume size or shape. LeBlanc used 5 particles per cell in his study (Reference 18). So the our study used NPTPND = 5 for most runs.

4. Rainfall Recharge Rate

The rainfall recharge rate, RECH(I,J), was varied ±20 percent, a wider variation than necessary since this is a long-term climate parameter. Rainfall can vary appreciably over a few months, or even a few years. But forty-year averages, as used in this study, tend to have less than ±20 percent variation.

Over the area of the aquifer, rainfall is the largest source of groundwater, significantly larger than the sewage flow. Due to the source and sink boundary conditions at Ashumet Pond, rainfall has an interesting effect. Increased rainfall tends to wash more contaminated water out through the sink cells in Ashumet Pond. The mechanism was explained in the calibration section. Without the loss of solute at the pond, increased rainfall would dilute the plume and increase its extent. With the loss of solute at the pond, increased rainfall dilutes the plume and reduces its extent.

Results were obtained for three variations in rainfall rates. The results of a 20 percent increase are shown in Figure 43, 20 percent decrease in Figure 44, and a tenfold increase in Figure 45. Dilution was so great in this last case that the comparable pollution contours only indicate a small plume area between the sand beds and Ashumet Pond being contaminated. LeBlanc wrote in his report (Reference 18) that the ratio of hydraulic conductivity to net rainfall recharge was just as important as the two

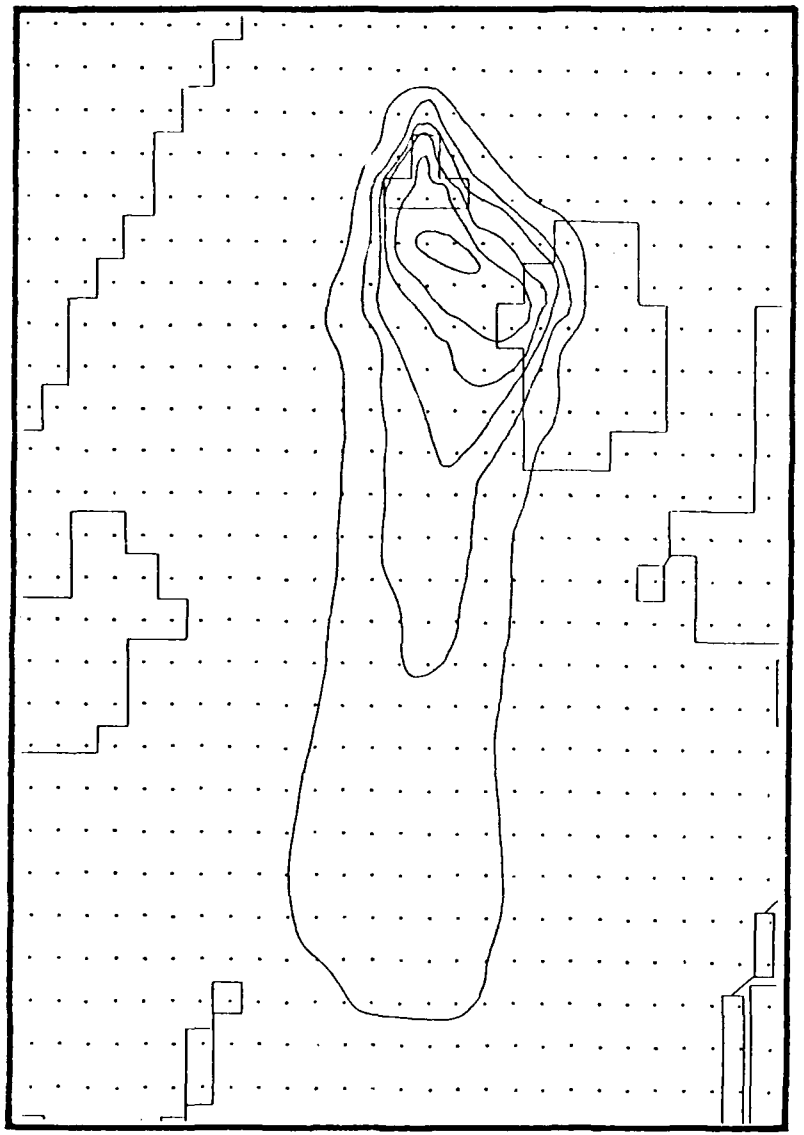

Figure 43. USGS-2D/Otis Plume Concentration Map for a Rainfall Rate Which is Increased by 20 Percent.

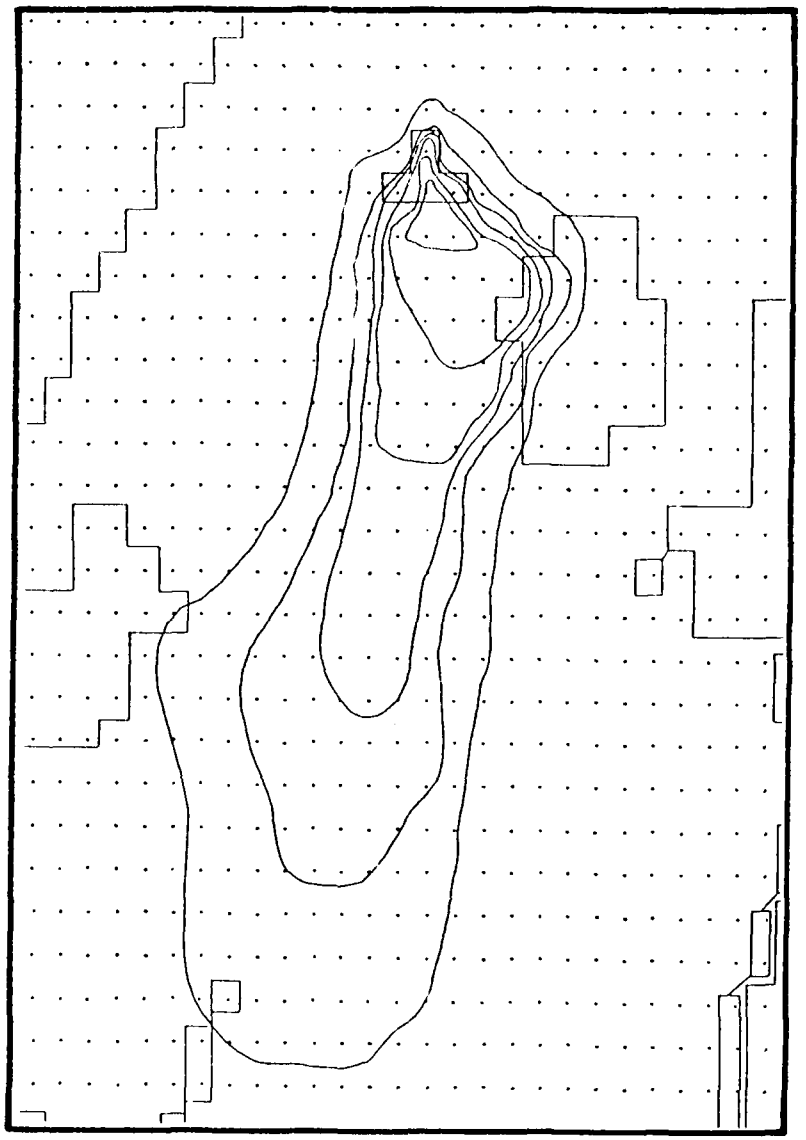

Figure 44. USGS-2D/Otis Plume Concentration Map for a Rainfall Rate Which is Decreased by 20 Percent.

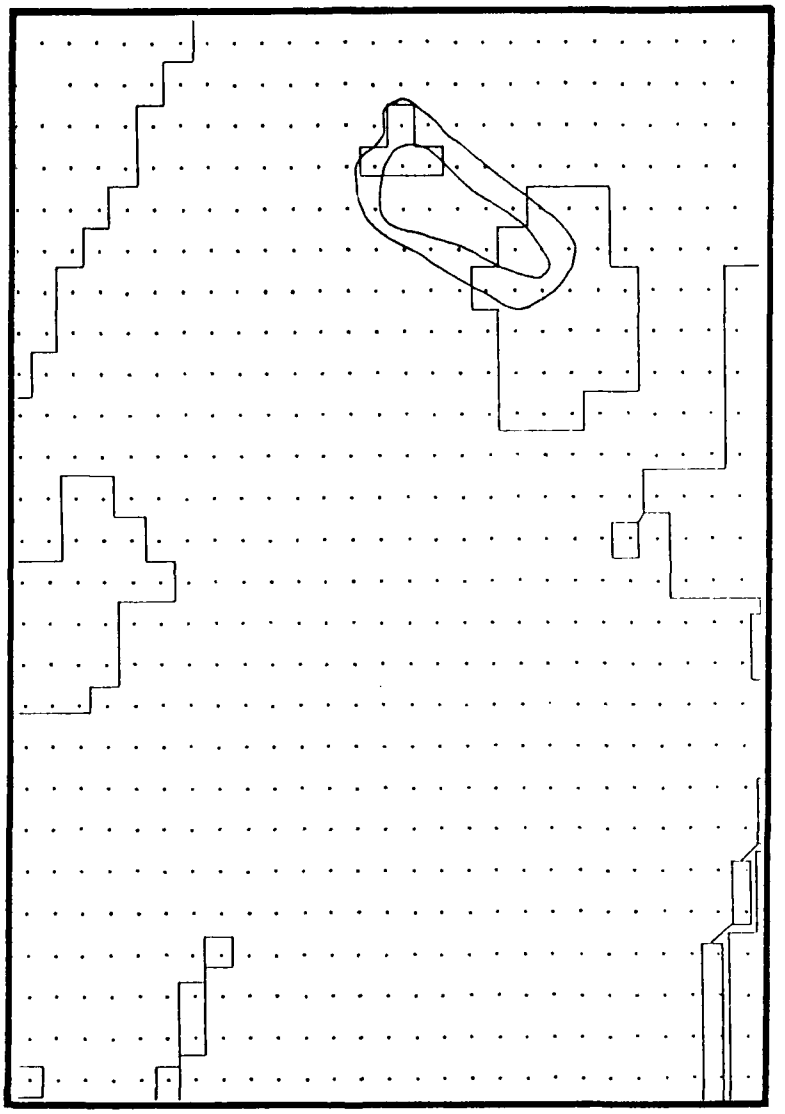

Figure 45. USGS-2D/Otis Plume Concentration Map for the Base Case Rainfall Rate Increased Tenfold.

individual values. However, the current study did not test this particular result.

5. Solute Concentration in Sewage Flow

The concentration of solute in the sewage flow, CNRECH (I,J), was adjusted by ±20 percent. This adjusted the concentration proportionately at any point within the plume, see Figures 46 and 47.

6. Longitudinal Dispersivity

Longitudinal dispersivity, BETA, was varied from 0 to 100 feet. Increasing dispersivity appears to blur the edges of the plume. It did not appear to have any other major effects. However, the results were best with BETA in the range from 40 to 100 feet, see Figures 48 and 49. As LeBlanc found, there was no appreciable change between 40 and 100 feet.

The cell size chosen by LeBlanc may be too large to show dispersional effects properly. The dispersion coefficients might visibly affect the results if the discretization of the aquifer was fine enough. The SUTRA manual (Reference 8) recommends XEDL ≤ 4(DISPL) and YDEL ≤ 4(DISPL). The CYBER system is too small for this fine a discretization at Otis. Fortunately, dispersional effects are not critical to the current use of the USGS-2D simulation.

7. Transverse Dispersivity

Transverse dispersivity, DLTRAT, is usually 0.1 to 0.5 times the longitudinal dispersivity. The effects of this variation were noticeable, but not extremely strong, see Figures 50 and 51.

8. Sewage Flow Rate

Increases and decreases in sewage flow rate, SWGFLO, proportionately increased and decreased the flow of water and solute into the sand beds. The results were basically as expected, as seen in Figures 52 and 53.

9. Leakance Coefficient at Ashumet Pond

Changes in the leakance coefficient were initially ±20 percent. This made no visible difference in the pollutant plume. Even a small effect, if it existed, would probably be visible in USGS-2D runs. In the USGS-2D model, cells with leakance coefficients greater than 1E-5 are treated as constant head cells. When the leakance coefficients were reduced by 88 percent, there was only a slight change in the plume. When the leakance coefficients were reduced by 97 percent, a major change occurred (Figure 38). In this last case, leakance into and out of Ashumet Pond was greatly reduced, as were the pond's effects on the plume. This phenomenon was discussed in the calibration section.

10. Pond and River Levels

LeBlanc published pond levels, but not river levels. He used

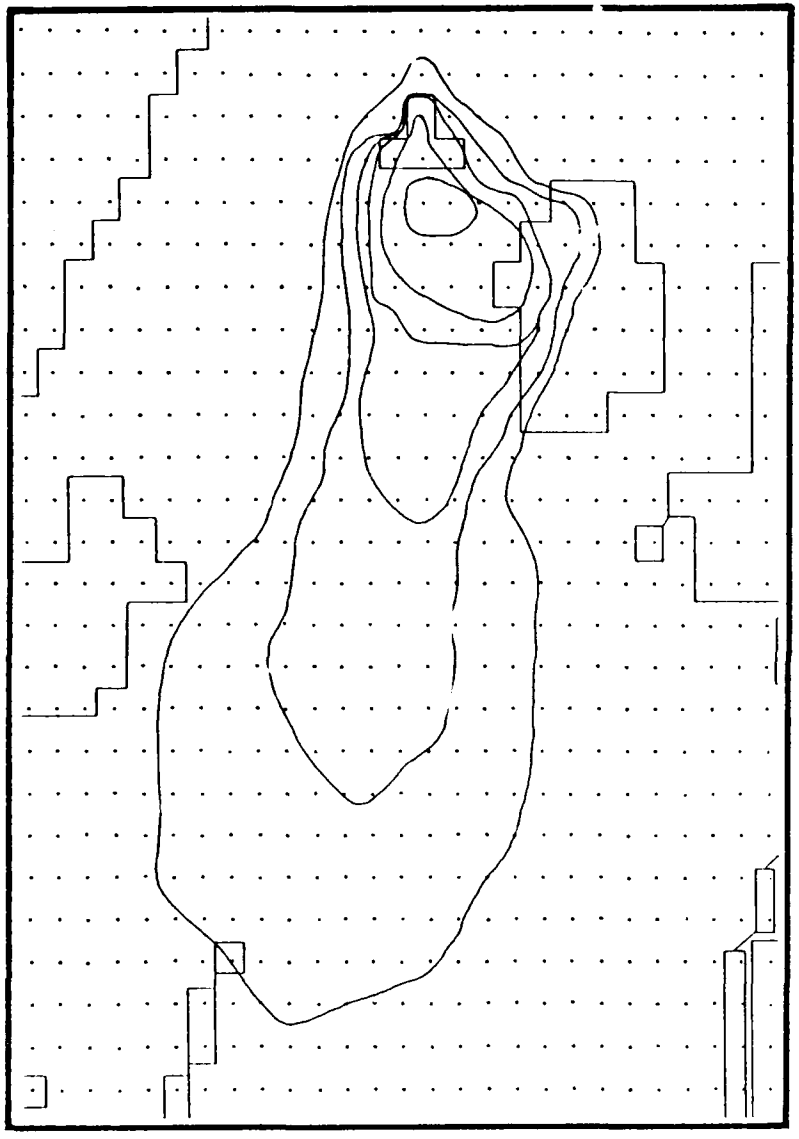

Figure 46. USGS-2D/Otis Plume Concentration Map for a Boron Concentration of 600 ppb at the source.

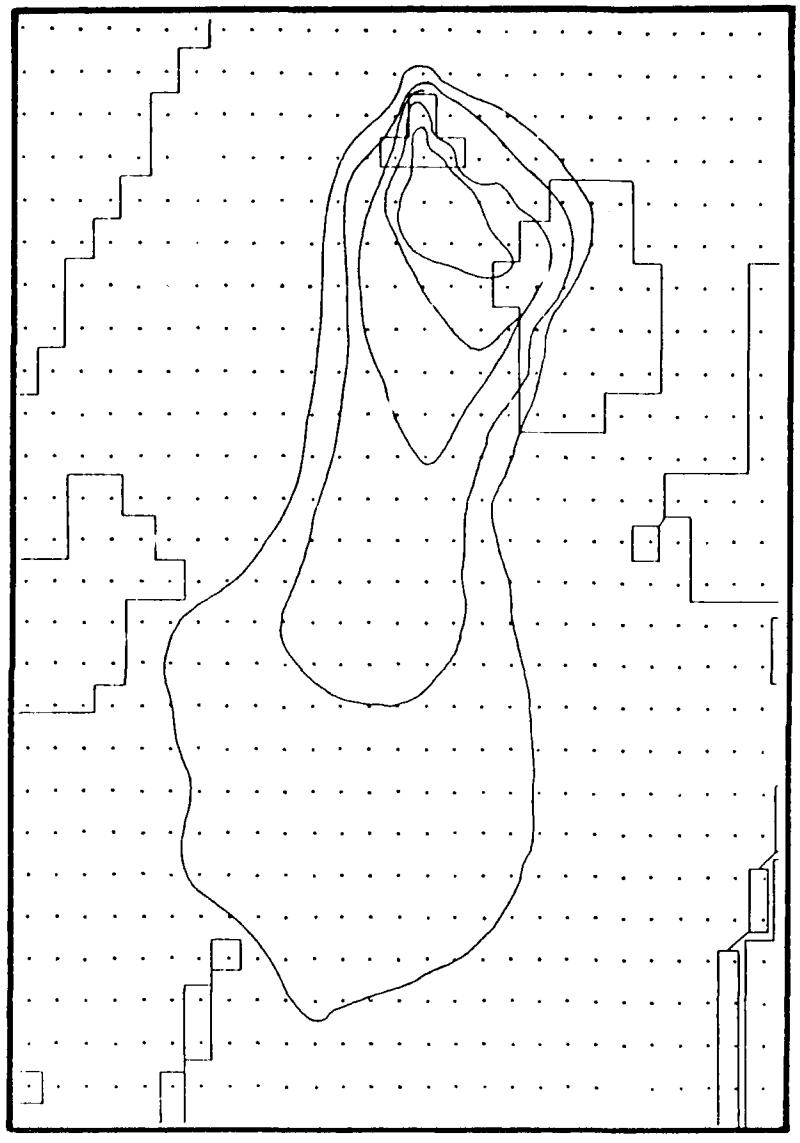

Figure 47. USGS-2D/Otis Plume Concentration Map for a Boron Concentration of 400 ppb at the Source.

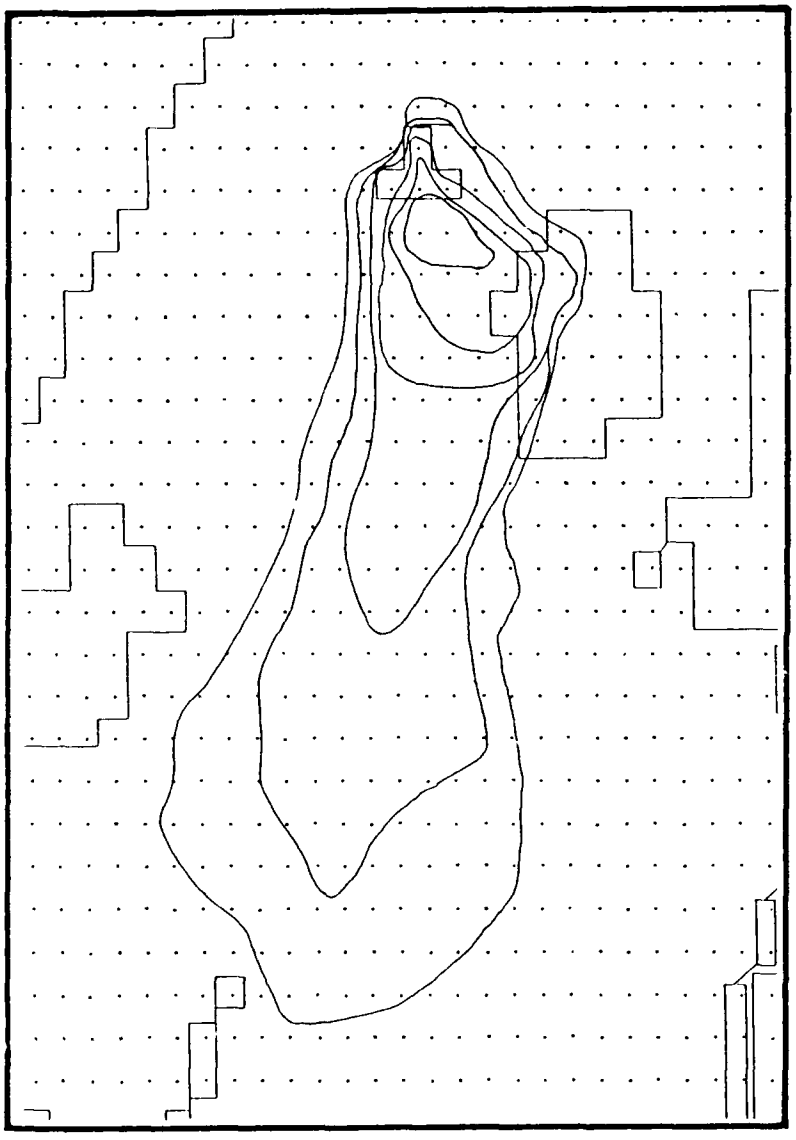

Figure 48. USGS-2D/Otis Plume Concentration Map for BETA = 0.01 Feet.

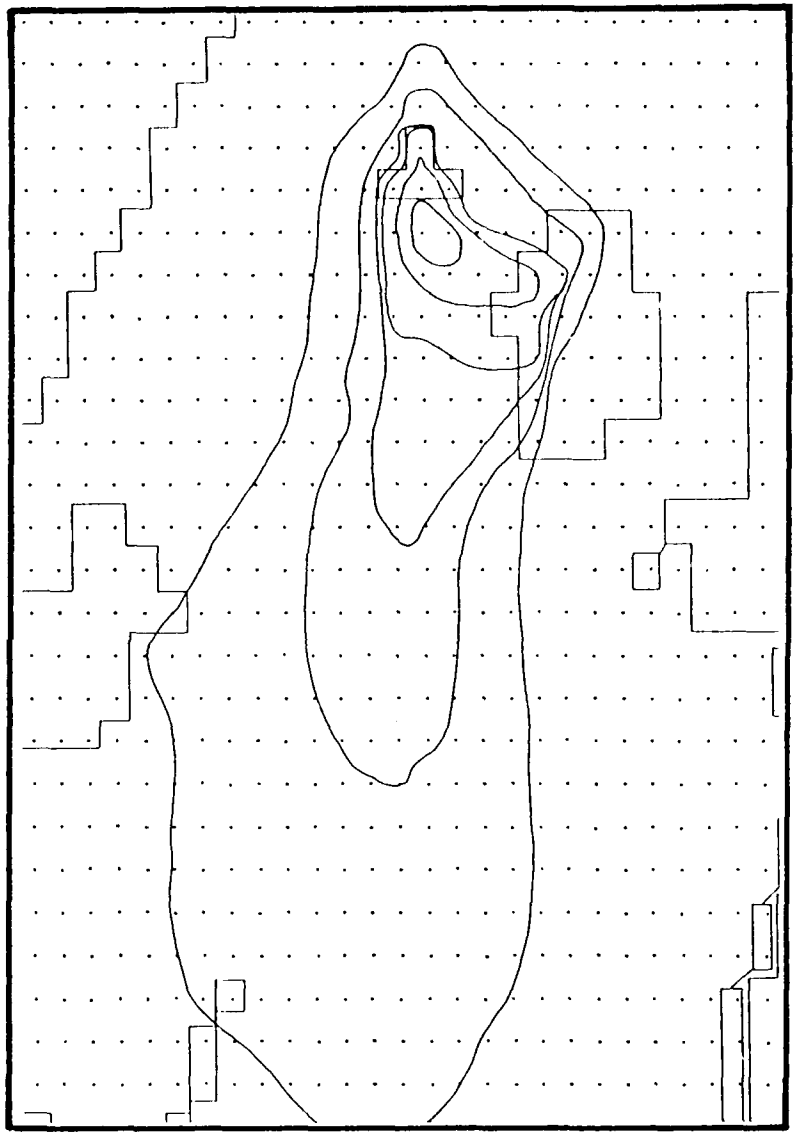

Figure 49. USGS-2D/Otis Plume Concentration Map for BETA = 100 Feet.

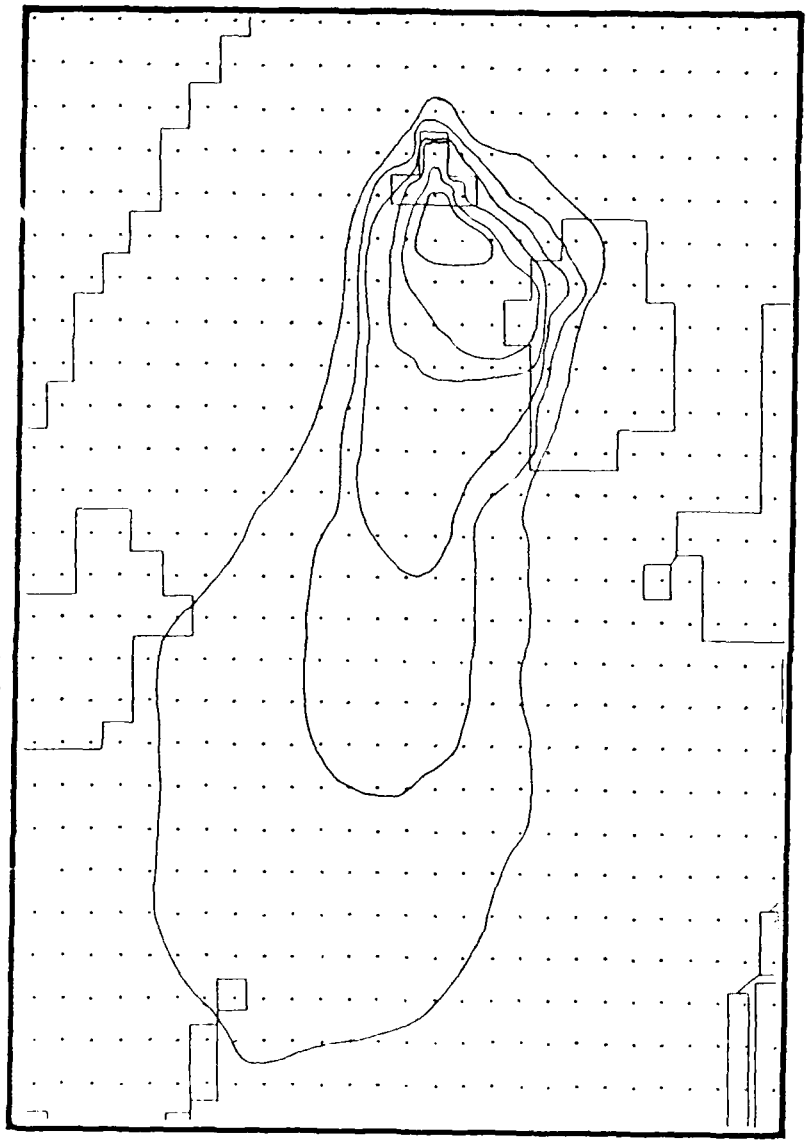

Figure 50. USGS-2D/Otis Plume Concentration Map for DLTRAT = 0.50.

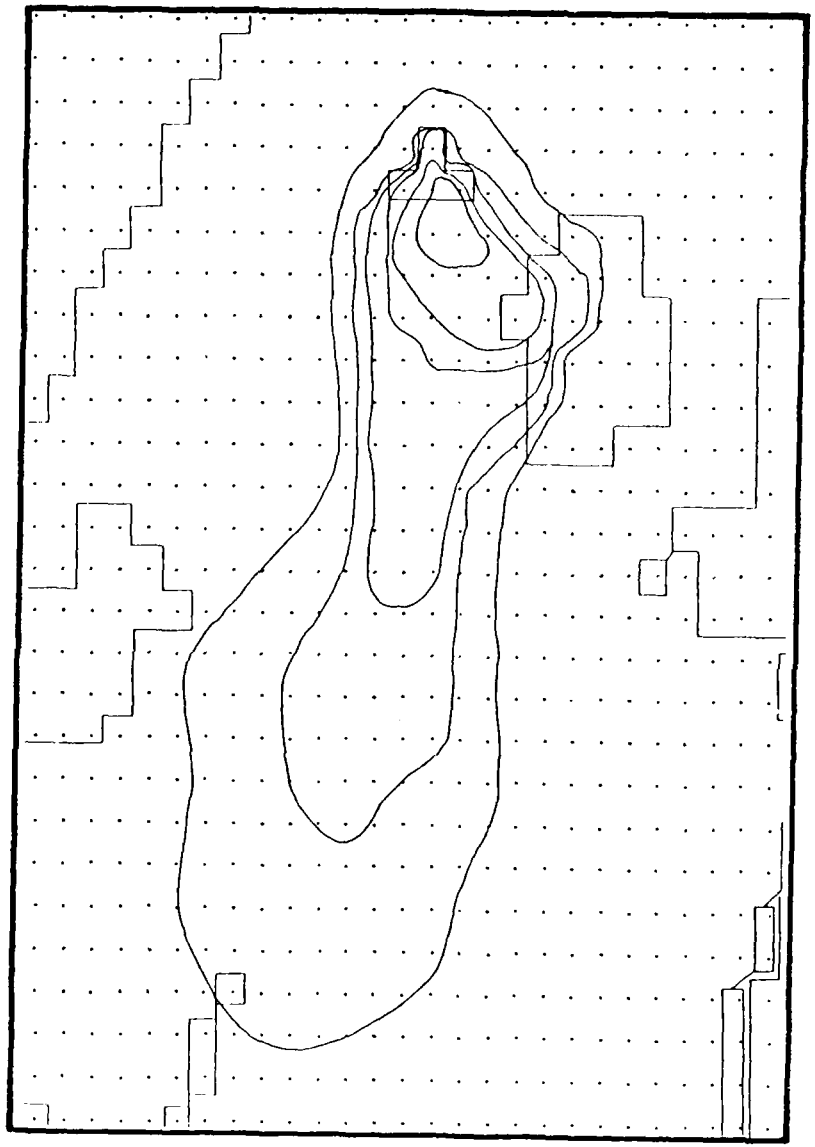

Figure 51. USGS-2D/Otis Plume Concentration Map for DLTRAT = 0.10.

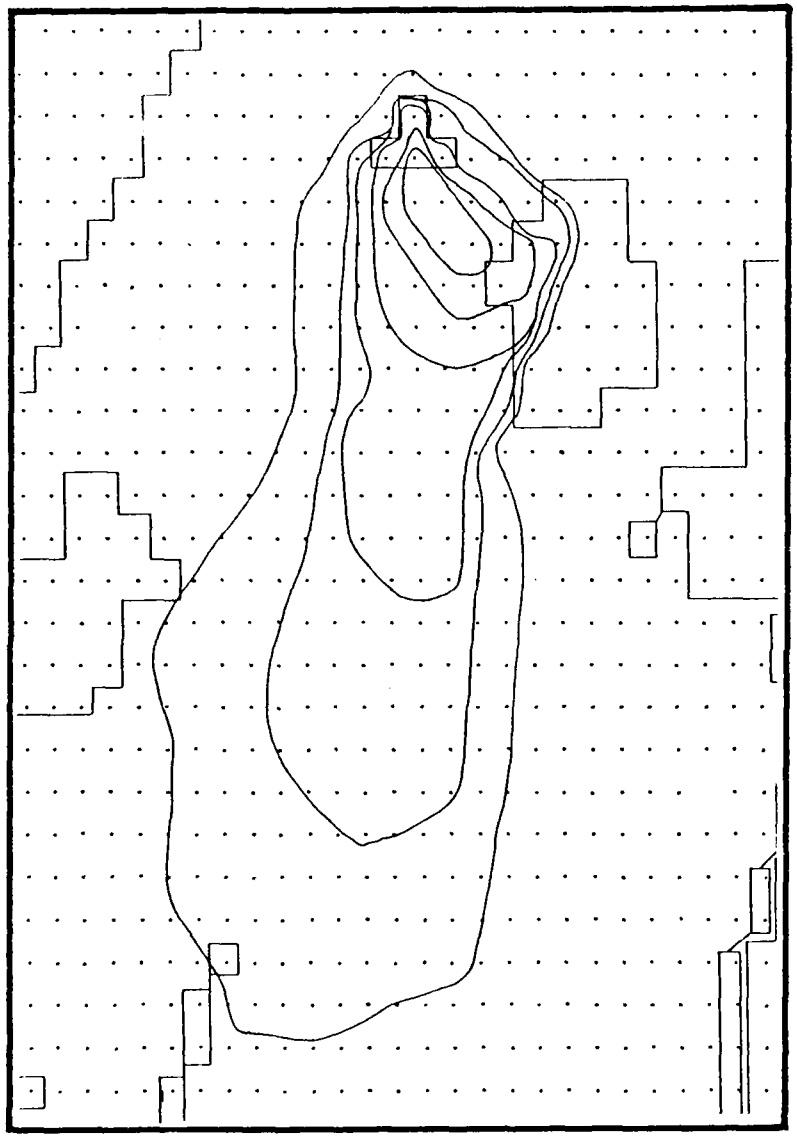

Figure 52. USGS-2D/Otis Plume Concentration map for SWGFLO Increased 20 Percent.

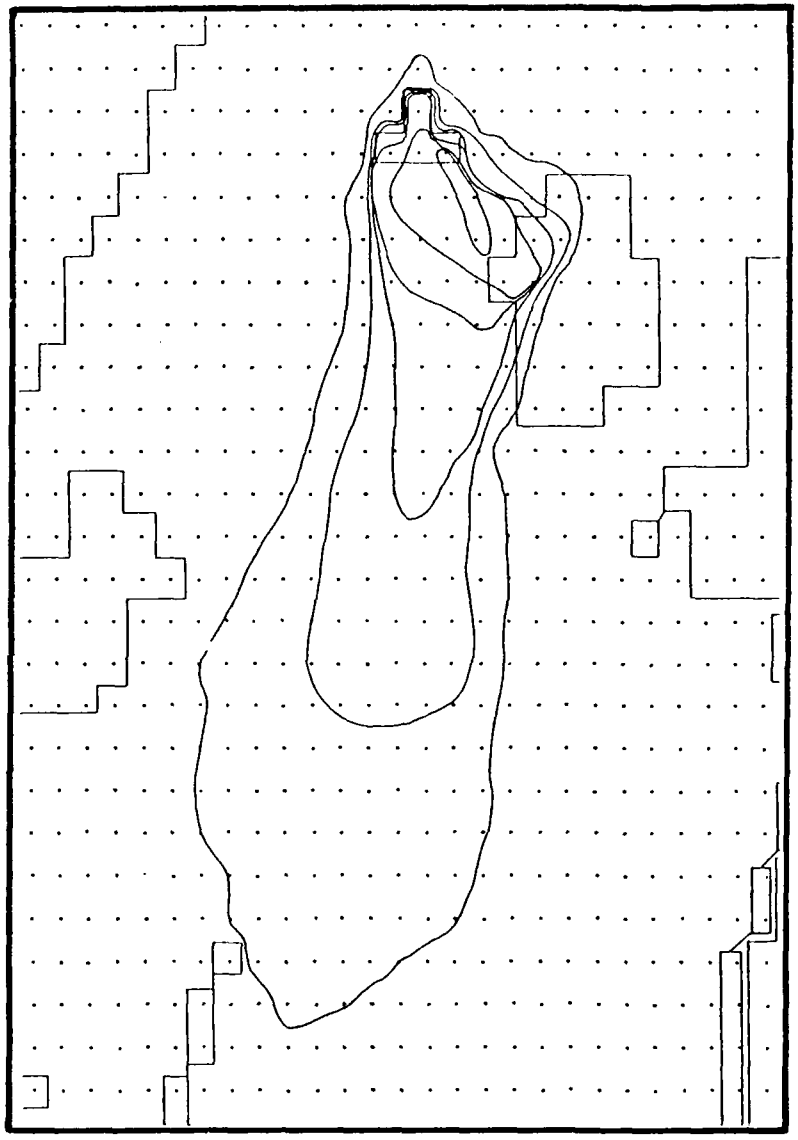

Figure 53. USGS-2D/Otis Plume Concentration Map for SWGFLO Decreased 20 Percent.

topographic maps to set the river levels. In our base case, LeBlanc's published pond levels were used and river levels were simulated as approximately linear between the relevant pond levels and the 10-foot water table contour at the lower (southern) end of the domain of computation.

Pond levels and other water levels were adjusted in the sensitivity study. In two of the sensitivity runs, water levels were tilted to the east and to the west. Tilting toward the west means slightly lowering (by 4 inches) the levels in Coonamessett Pond and River, and slightly raising flow rates toward the east in Johns Pond and the Childs River. The effects of this "tilting" were minor.

11. Backus River Node Boundary Condition Levels

The head boundary values of the Backus River cells were changed moderately. However, this only visibly changed the plume's shape in the cells near the river, which is the southern end of the plume where it is rather dilute.

12. CELDIS

CELDIS is the maximum distance that a particle can travel before its velocity is recalculated based on its new position. The base case value is 0.50. Values of 0.25, 0.75, and 1.0 were also considered. Most of the particles are affected by changes in CELDIS, the faster-moving particles being affected more than the slower ones. The average particle velocity is about 1 ft/day. Typical particle velocity ranges are from 0.5 to 2.0 ft/day. The maximum particle movement interval is 4 years (1461 days). Therefore, for CELDIS = 0.5, most particles will have their velocities recalculated at least once during a 4 -year time increment for 750 ft N-S cell lengths. It is more efficient to reduce CELDIS than to shorten the time increment. Particle velocities should be recalculated only when necessary.

13. Anisotropy Factor for Hydraulic Conductivity

ANFCTR is the anisotropy factor for hydraulic conductivity, where transmissivity is specified in the xx (E-W) direction as Txx = (hydraulic conductivity) (saturated thickness) and in the yy (N-S) direction, as Tyy = (Txx) (ANFCTR). Increasing ANFCTR decreases the north-south hydraulic gradient, as expected. The groundwater flow required to maintain a steady state is proportional to ANFCTR times the hydraulic gradient. Increasing ANFCTR from 0.8 to 1.0 increases the length of the pollutant plume. Increasing ANFCTR from 1.0 to 1.2 noticeably increases both the length and the breadth of the plume, see Figures 54 and 55.

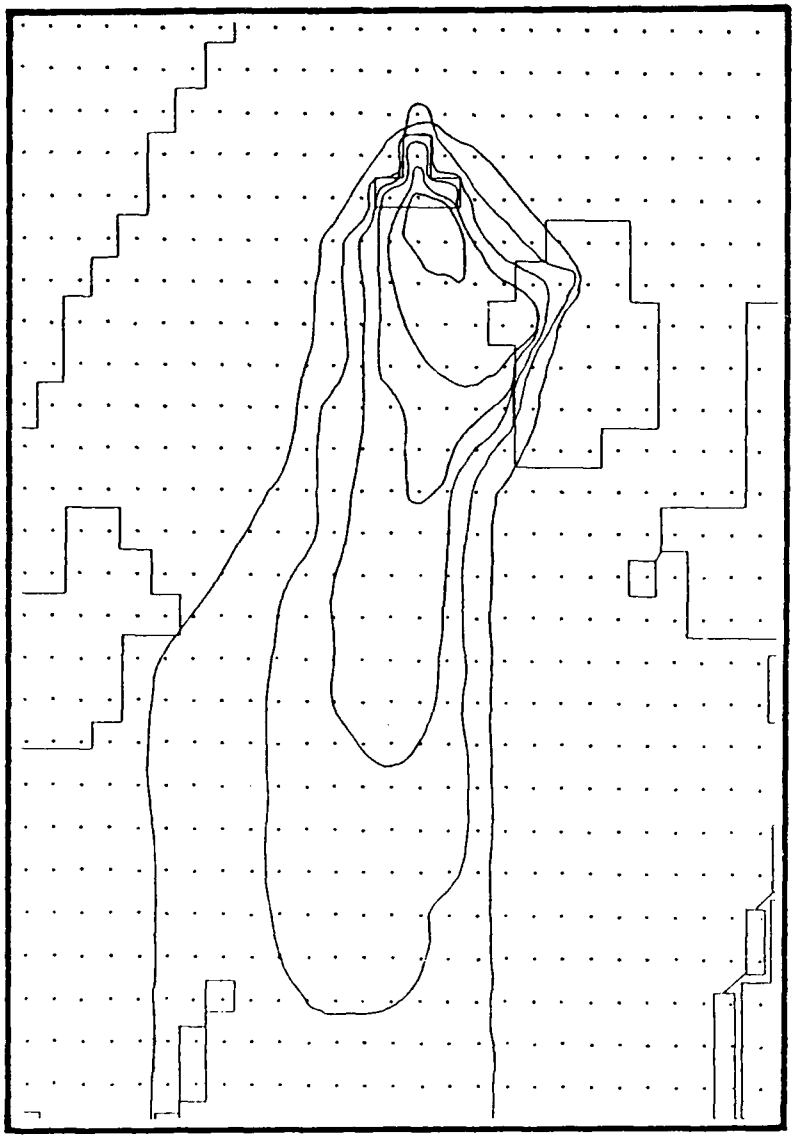

Figure 54. USGS-2D/Otis Plume Concentration Map for ANFCTR = 1.20.

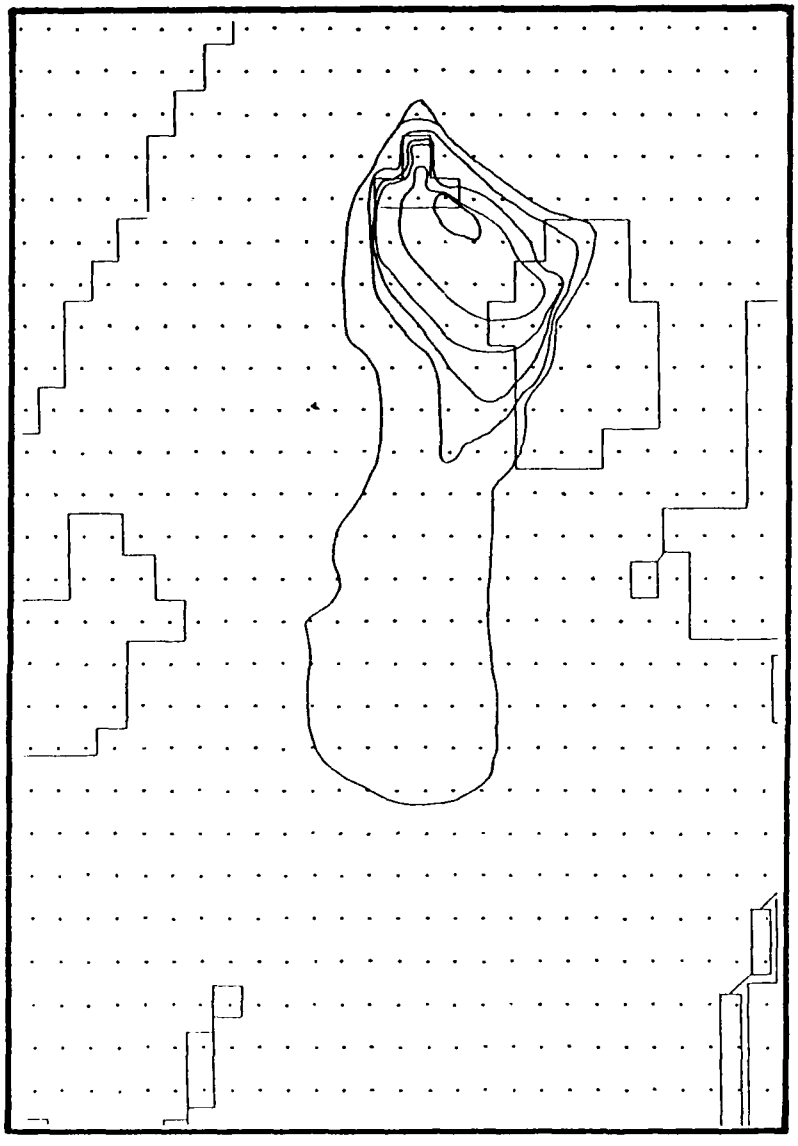

Figure 55. USGS-2D/Otis Plume Concentration Map for ANFCTR = 0.80.

SECTION VII

SIMULATION RESULTS USING THE RANDOM WALK MODEL

A. INTRODUCTION

Modeling efforts using the Random Walk (RW) program involved four major phases. Since the source program had previously been installed on the CYBER system, phase one was Preparation. In this phase the aquifer discretization was chosen, the input data file was prepared, and the necessary source code arrays were appropriately redimensioned. The second phase consisted of Implementation, where standard familiarization/test cases were run and problems were corrected, as needed, to permit complete, successful runs of the program. For example, one fatal data format error, caused oscillations in the head solver algorithm that resulted in unstable Otis simulation runs. In phase three, Calibration, several typographical errors were corrected, sink boundary conditions were adjusted, the dispersivity was increased, and other boundary conditions were checked. Finally, in the Sensitivity Study phase, 18 parameters were tested. Plume maps are given in this section for all parameters with noticeable sensitivity effects.

B. PREPARATION AND IMPLEMENTATION

1. Preparation Phase

The first step in the simulation was the preparation of the input data file for the Otis sewage plume. An annotated input data file template is given in Appendix E. Input parameter values were taken from LeBlanc's published data wherever possible. The units from the USGS-2D data file were converted from a (ft^3-ft sec) basis to the Random Walk (gal-ft-day) basis. The values based on LeBlanc's work are shown in Table 9. The other values, deduced from the User's Manual (Reference 6) or from empirical testing, are shown in Table 10.

2. Implementation Phase

The source program had already been implemented on the CYBER computer system; however, system updates were incorporated in the various files. Then, sample problems from the User's Manual (Reference 6) were run. Problems No. 1,3,4,5 were straightforward. Problem 2 was more complex. It ran properly, but it took considerable time to fully interpret the results. Full interpretation was required to know that the problem was running properly.

Next, LeBlanc's discretization grid (see Figure 34) and his input parameters from the USGS-2D format (see Tables 6,7) were adapted to the Random Walk format, as given in Figure 56 and Tables 9 and 10. However, when the Otis data file was run, instability problems were encountered. In the vicinity of Ashumet Pond, the head levels oscillated rather than converging. In an attempt to eliminate this oscillation, a number of parameters were varied. While the severity of the oscillations was reduced, it was not completely eliminated.

The input data formats in the User's Manual were rechecked. The interpretation of the constant-head cell input parameters may have been the

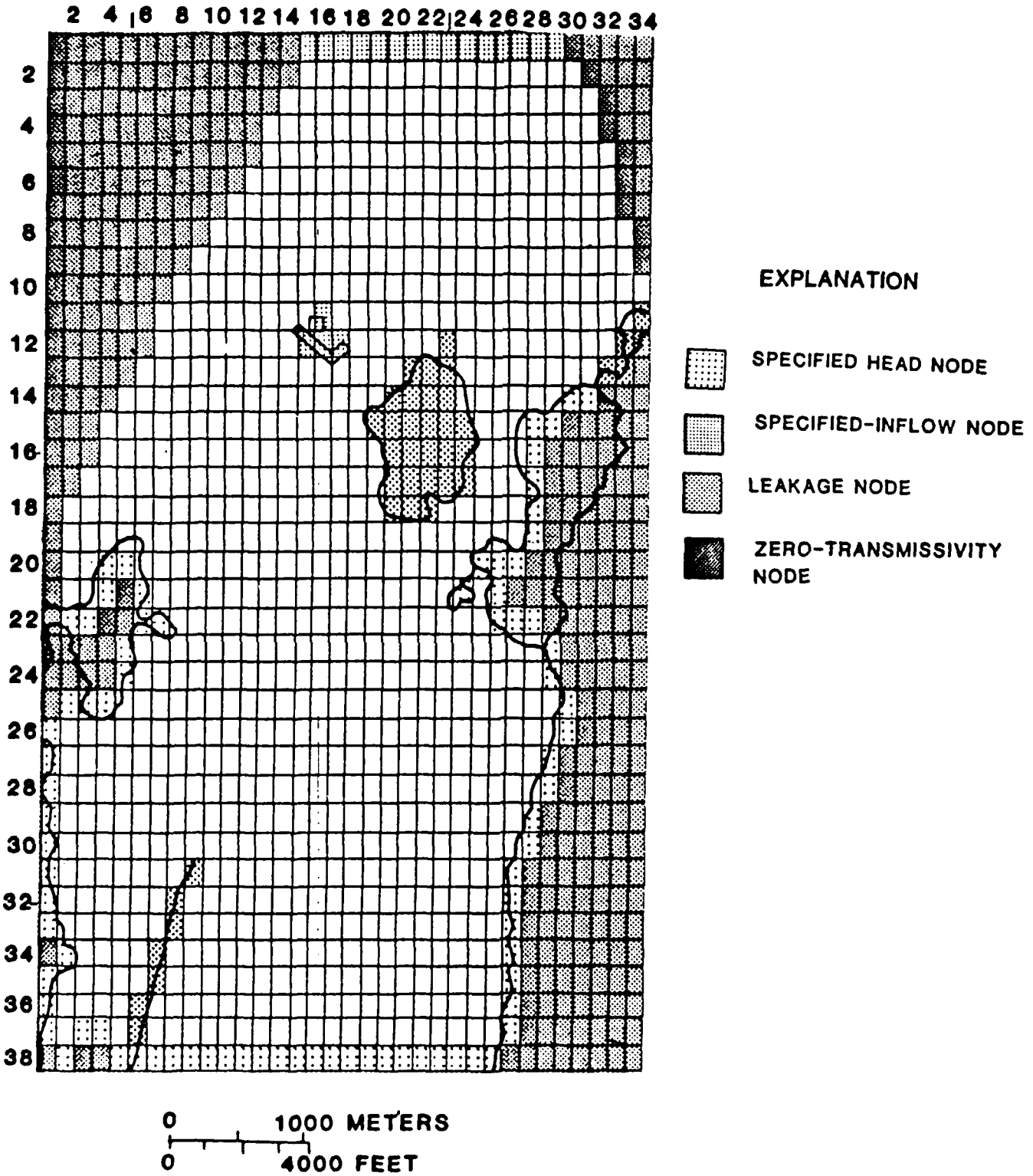

Figure 56. Grid for the Random Walk Simulation of the Otis Sewage Plume.

TABLE 9. LEBLANC'S PUBLISHED INPUT PARAMETERS ADJUSTED FOR THE RANDOM WALK SIMULATION OF THE OTIS SEWAGE PLUME (AFTER REFERENCE 17).

INPUT PARAMETER	VALUE
NC = number of columns in aquifer grid.[a]	34
NR = number of rows in aquifer grid.[a]	38
Default Values Card [b]	
NPUMP = number of pumps	0
DELX = width of a cell (all I,J) [c] [d]	500.
DELY = length of a cell (all I,J) [c] [d]	750.
DISPL = longitudinal dispersion coefficient (Later increased to 125.')	40.
DISPT = transverse dispersion coefficient (Later increased to 40.')	13.
EPOR = effective porosity	0.35
APOR = volumetric porosity[e]	0.35
RD1 = Retardation factor[f]	1.0
KD = Consistent with RD1 = 1[g]	0.0
Q(i,j) = Net recharge/evapotranspiration	[h]
R(i,j) = Leakance coefficient	[h]
RH(i,j) = surface elevation of pond[i]	[h]
RD(i,j) = elevation of bottom of resistance layer to flow [i] (in this case, the bottom of the pond sediment layer)	[h]
CH(i,j) = elevation of top of aquifer [i]	[h]
PERM1(i,j) = permeability of cell, Y direction	[h]
PERM2(I,J) = permeability of cell, X direction	[h]
BOTT(i,j) = elevation of bottom of aquifer cell [i]	[h]

---

a NO impermeable boundary along edges of aquifer

b Because over half of the permeable cells required boundary condition specifications on node cards, a node card was prepared for each cell. Therefore, no values on the Default Value Card, except NC & NR, will actually be used.

c See corresponding array map for the USGS-2D/Otis simulation, Figure 34

d Because of the time required to rediscretize the mesh, the mesh size was never changed to check its effect on the solution.

e NOTE that EPOR ≤ APOR.

f LeBlanc modeled Otis successfully without using retardation or adsorption. The solute (i.e., boron) seldom adsorbs on sand and gravel particles. An input value of 0.0 will default to 1.0.

g When KD = 0, RD1 = 1.0 (NO adsorption).

h See the array map in the "node card deck".

i Elevation in feet above mean sea level

TABLE 10. INPUT PARAMETER VALUES FOR THE RANDOM WALK SIMULATION OF THE OTIS SEWAGE PLUME, DEDUCED FROM REFERENCE 6 AND EMPIRICAL TESTING.

Values Deduced From User's Manual			
NSTEPS	=	total number of time increments in head solution	1
ERROR	=	convergence tolerance of head solver algorithm (recommended value for steady-state flow) [ft]	0.10
NRT	=	number of pumpage periods (no pumps)	1
H(I,J)	=	initial head map of cells (has no effect on steady-state flow cases)	a, b
IP, JP	=	Pump coordinates. In this case, the only pump is a dummy pump, with zero flow.	
P1	=	Pump flow rate [gal/day]	0.0
X1	=	X position of upper left corner of rectangular source in subroutine GENP(PL).	c
Y1	=	Y position of upper left corner of rectangular source in subroutine GENP(PL).	c
DX	=	Width of rectangular sources in GENP(PL).	c
DY	=	Length of rectangular source in GENP(PL).	c
PL	=	Rate of solute [lb/day] supplied by source GENP(PL).	
RHO	=	Specific gravity of grains in solid matrix. (Approximate value for quartz & feldspar.)	2.6[d]
Values Deduced from Empirical Testing			
DELTA	=	the length of a head solver, or GW flow, time period [days]. (User's manual recommends this value for steady state simulations)	1.0E10
NPITS	=	particle advance iterations per GW flow period.[e]	80
SF1(I,J)	=	artesian cell storativity.[f]	1.0E-4
SF2(I,J)	=	storativity of water table cells, approximately equal to porosity[g]	0.35
NSP	=	number of time increments per pumpage period.[h]	2
DELP	=	the time increment of a particle move period in days.	182
MAXP	=	maximum number of particles allowed.[i]	9000
PM	=	Pounds of solute per particle.[j]	3545.
MARK(i,j)	=	The identification number of the sink with which a sink node is associated.	k
CONSOR(i,j)		Source concentration [ppm].	l
DXMAX, DYMAX			m

TABLE 10. INPUT PARAMETER VALUES FOR THE RANDOM WALK SIMULATION OF THE OTIS SEWAGE PLUME, DEDUCED FROM REFERENCE 6 AND EMPIRICAL TESTING (CONCLUDED).

a Elevation in feet above mean sea level.

b See aquifer map, Figure 56.

c Because GENP(PL) is not used in Otis simulations, the values specified are unimportant. Subroutine GENP(PL) has effectively been turned off by specifying a negligibly low value of solute injection rate, PL. The units are call index number (dimensionless).

d Not used by the program, because RD1 is never calculated.

e A balance between increased run time and increased extrapolation errors in particle movements.

f Started with the value from the sample problems in the User's Manual, and checked later to confim the lack of visible effect during the sensitivity runs.

g Initially used the value from the sample problems in the Users' Manual for water table cells (i.e., 0.10). Later corrected it to the aquifer porosity (i.e., 0.35).

h In a steady-state flow case, there is no obvious logical reason not to use 1, and the Otis sensitivity study appears to confirm this. However, the User's Manual, without explanation, uses NSP = 2.

i Started at 5000. Later increased to 7500 and 9000 for better definition in the dilute, southern portion of the plume.

j Started at 3545. Later reduced to 1700 for better plume definition.

k Particles will not leave the aquifer at a sink node unless a valid association is made on a sink location card. (Initial simulation attempts without these cards were not wholly successful.) The cards enable certain automatic particle/sink bookkeeping routines.

l Entered on Source Concentration Cards : I, J, CONSOR(I,J). Required for all cells containing a source of non-zero solute concentration.

m The fraction of a cell that a particle can move before its velocity must be recalculated at the new position. This parameter is not included in the input data set, but could be changed, before each affected run, directly in the source code.

source of the problem. Initially, it was assumed that if the water entering a constant-head cell had zero solute concentration, SF2 was set to 1.0330. For non-zero solute concentration, R(I,J) was set to 1.0E10.

By trial-and-error, it was found that for the non-zero concentration case, the user must set both

SF2 = 1.0E30 and R(I,J) = 1E10.

This permitted stable simulations.

3. Groundwater Flow Calibration

Little effort was required to calibrate the groundwater flow solution. The key parameter values were taken from the USGS-2D results. After the program converged for the Otis input data, several runs were used to correct typographical errors in the input data file. At this point, as expected, the water table map form the Random Walk model (Figure 57) closely matched the water table map from the USGS-2D simulation (Figure 35).

4. Solute Transport Calibration

First, solute sink location cards were specified as required since none had initially been included in the input data file. Without sink cards, no solute particles were captured by sinks, resulting in an excessive accumulation of particles and corresponding excessive simulated solute concentrations in Ashumet Pond after the 40-year simulation period. Thus, sinks were specified in the upper (northern) halves of Ashumet Pond, Johns Pond, Coonamessett Pond, and the Backus River. The lower halves of those bodies of water function as sources, rather than sinks. These sink specifications improved the fit of the simulated pollutant plume.

There is another important sink located at the southern boundary of the computational domain near the 10-foot water table contour line. This sink strongly affects the simulated head distribution, giving a reasonable comparison with field data. But, it does not affect the concentration distribution because no particles reach that sink with the 40-year simulation.

Near Ashumet Pond, the result of the added sinks was that too many particles were captured. In the USGS-2D simulation and in the field data, there were substantial solute concentrations in the aquifer cells under the northwest portion of Ashumet Pond. There were no particles under Ashumet Pond in the Random Walk simulation because the source coding requires that all particles be captured immediately upon entering sink cells. To correct this problem, it was necessary to change the particle capture coding. A scientifically rigorous but inconveniently complicated method would be an algorithm with 3-D particle tracking, allowing vertical leakage from the top of the cell. So, a shorter, more convenient method was set up, using an empirically derived hypothetical "capture zone." A particle near a sink node will be captured only if it enters the capture zone surrounding the node. This capture zone is an artificial entity; however, it can be adjusted empirically to yield fairly realistic results.

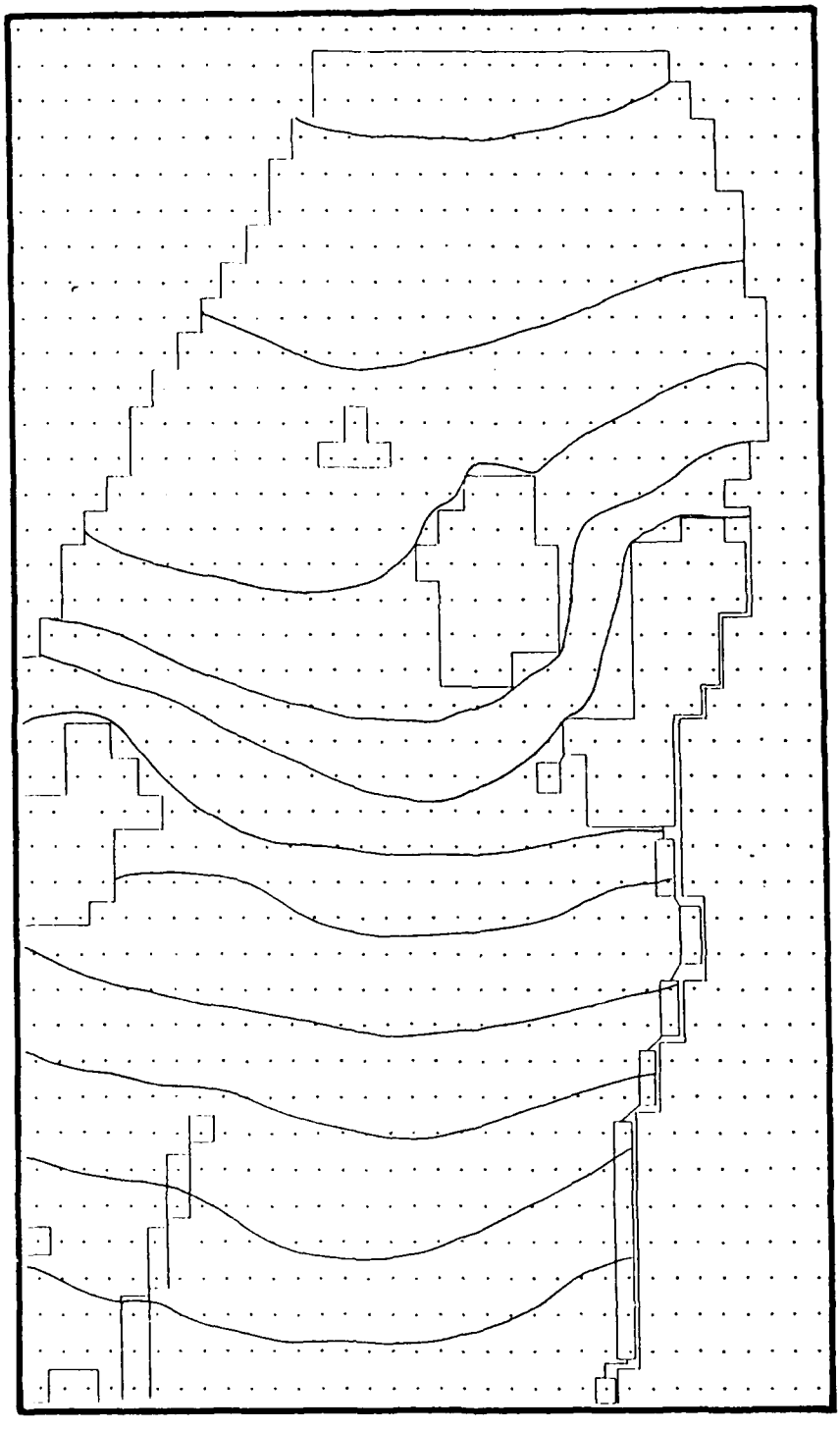

Figure 57. Simulated Water Table Contours Using the Random Walk Head Solver and Otis ANGB Data.

The capture zone was defined as an ellipse surrounding the affected node. The major and minor radii are (CPRD)(DELY) and (CPRD)(DELX), respectively. The numerical value of CPRD was varied from 0.20 to 0.60 in the calibration study, and from 0.40 to 0.525 in the sensitivity runs. The results of four CPRD sensitivity runs are shown in Figures 58 through 61. The optimum value was approximately 0.475.

DISPL is the longitudinal dispersion coefficient. In the USGS-2D simulation, DISPL was found empirically to be 40 feet to 100 feet. Within this range, the pollution plumes were not noticeably affected. In the current Random Walk simulations, DISPL was initially set at 40 feet. This resulted in the problem shown in Figure 62. That is, the western concentration contours of the simulated plume were shifted too far to the east of the corresponding contours derived from field data.

One explanation of this problem is that northwest of Ashumet Pond, the convective velocity turns nearly due east in grid rows 14 to 16. So for southeasterly traveling particles, the southern component of the velocity nearly disappears in these rows, while the eastward velocity component remains. Before the slow southward convection can carry many of these particles south to row 17, where the normal southward velocity resumes, eastward convection carries the particles into Ashumet Pond.

Consequently, runs were made with larger longitudinal dispersion coefficients. Better plume fits were found in these runs. One possible explanation is that the longitudinal dispersion carried many of the particles southward, through rows 14 - 16, before they were swept too far east by the convective currents.

However, this trial-and-error adjustment results in significantly larger dispersion parameters in the Random Walk model than used in the USGS-2D model. The optimal range of the longitudinal dispersion coefficient in the Random Walk/Otis simulations was found to be 100 to 150 feet. Numerical dispersion might explain the differences in this parameter between the two models for the Otis simulation.

Numerical dispersion is due to artificial smoothing of the concentration field by diffusive numerical algorithms. While the USGS-2D model was constructed to minimize numerical dispersion, the Random Walk method intrinsically has even less. The total dispersion is the sum of the dispersion due to the dispersion parameter and that due to numerical dispersion; thus, the specified dispersion coefficient in Random Walk should be increased to give results comparable to the calibration results of the USGS-2D model.

At this stage in the RW calibration, there was still an apparent discrepancy in the material balance. So, two geometric adjustments were tested. First, the sewage sources (i.e., those in the sand beds) were moved slightly away from Ashumet Pond, as shown in Figure 63. This was done in hopes of reducing solute losses in the Ashumet Pond sink cells. As shown in Figure 63A, the base case simulation of the sand beds uses four source cells. An alternate simulation used three source cells, shifting sewage flow from the easternmost source cell to the other three cells. This is shown in Figure

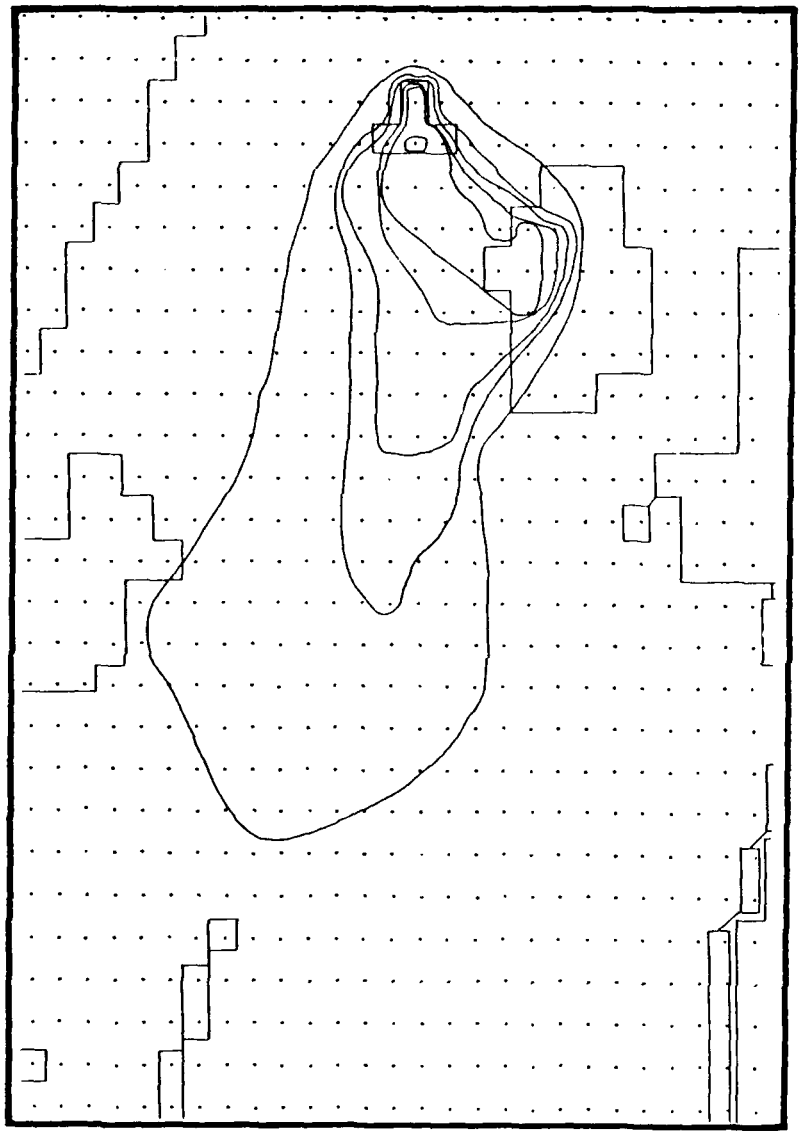

Figure 58. RW/Otis Plume Concentration Map for the Parameter CPRD Equal to 0.400.

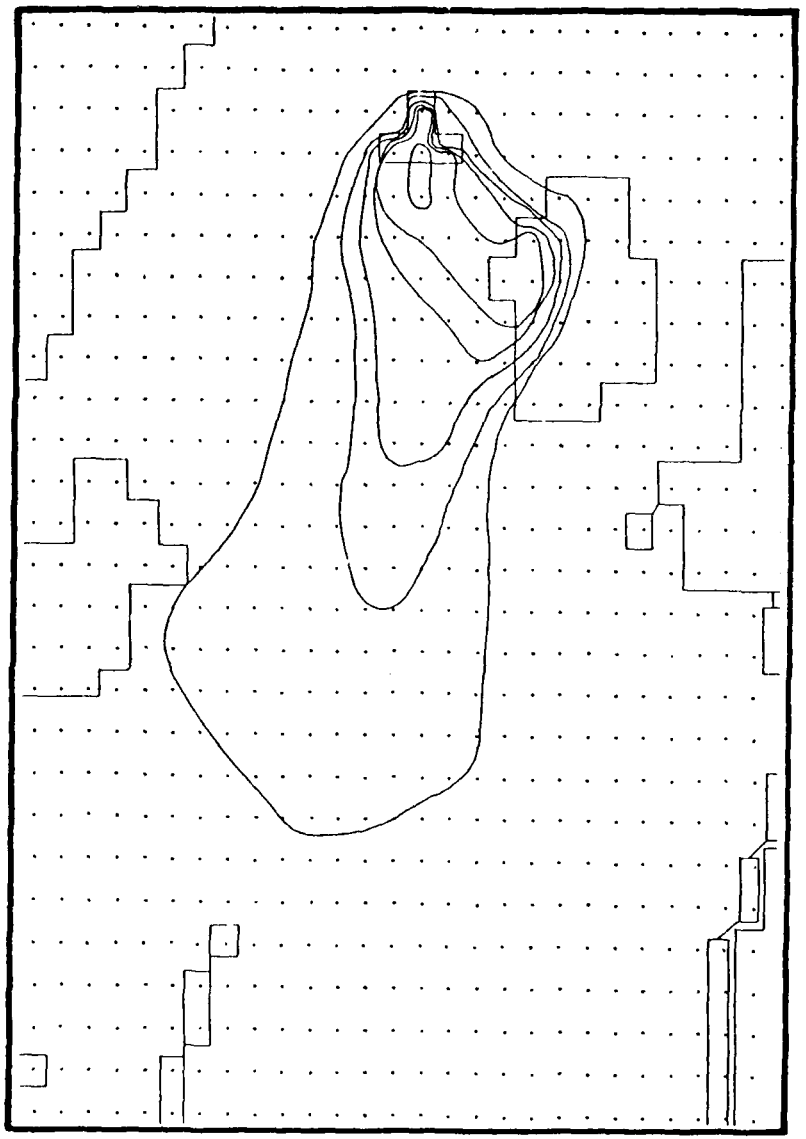

Figure 59. RW/Otis Plume Concentration Map for the Parameter CPRD Equal to 0.450.

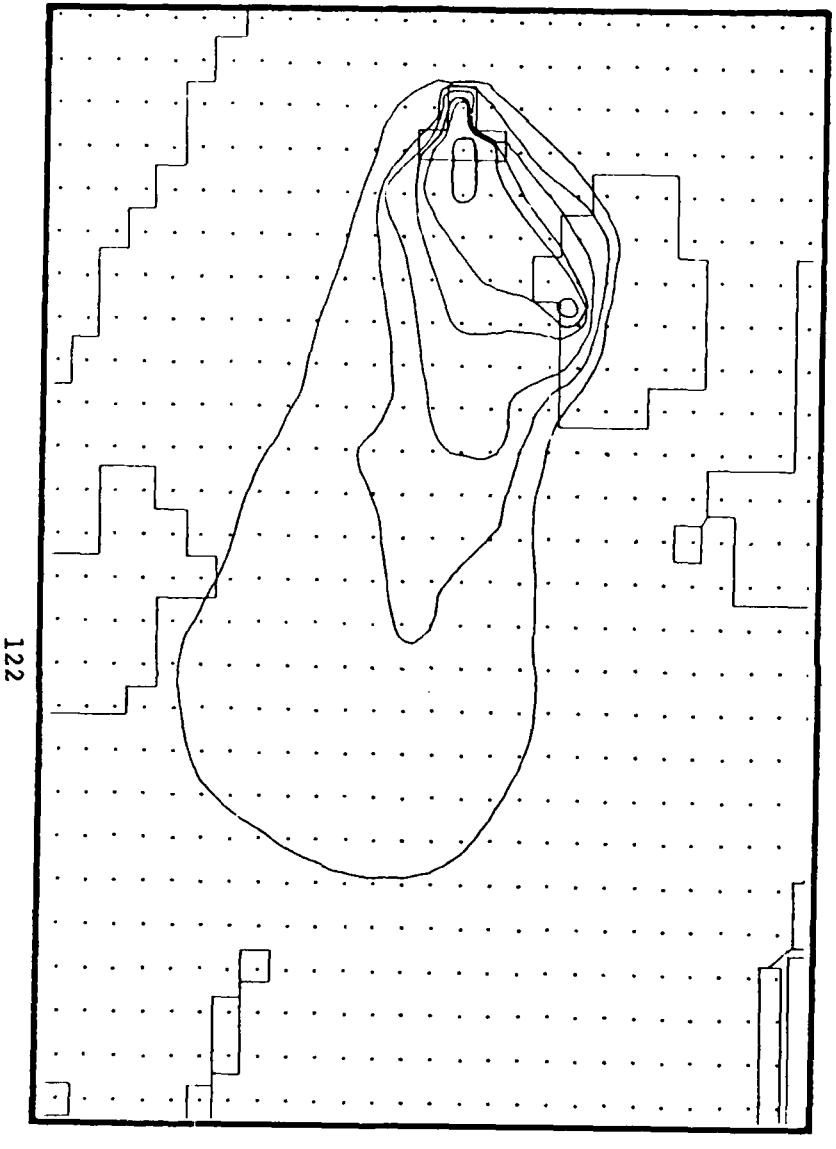

Figure 60. RW/Otis Plume Concentration Map for the Parameter CPRD Equal to 0.500.

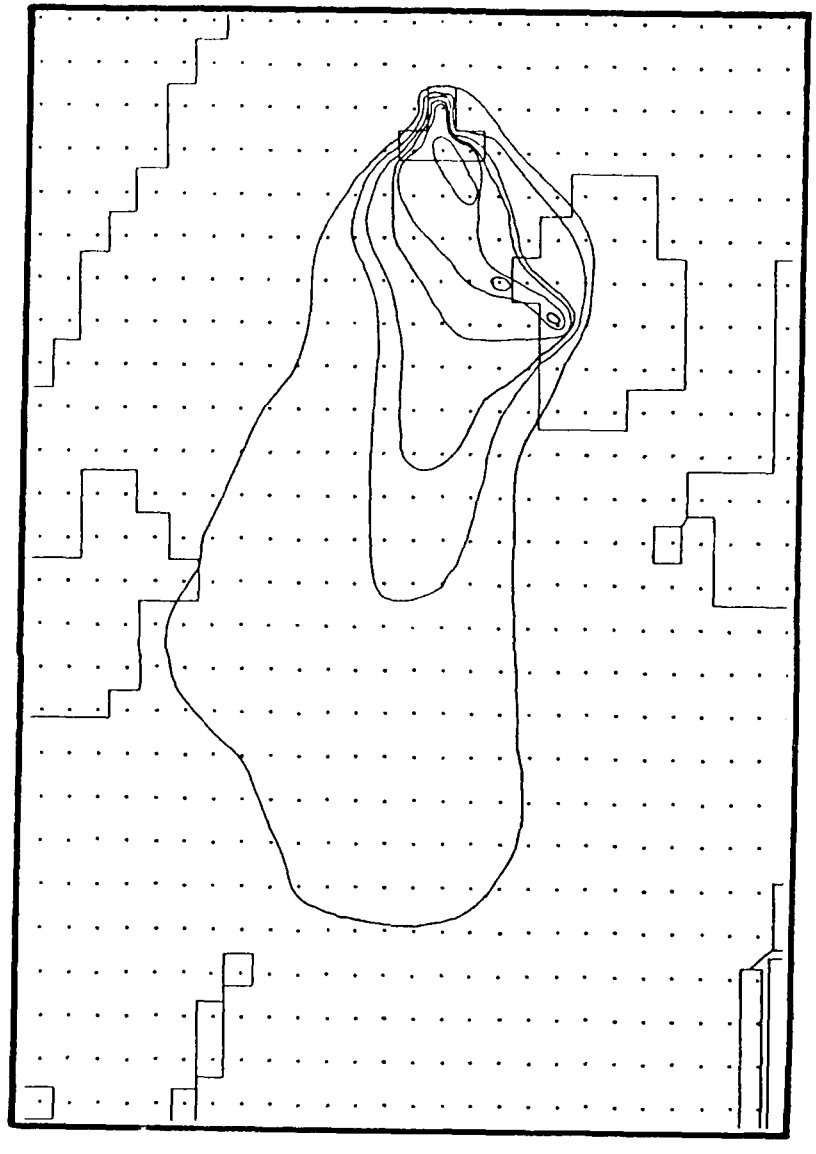

Figure 61. RW/Otis Plume Concentration Map for the Parameter CPRD Equal to 0.525.

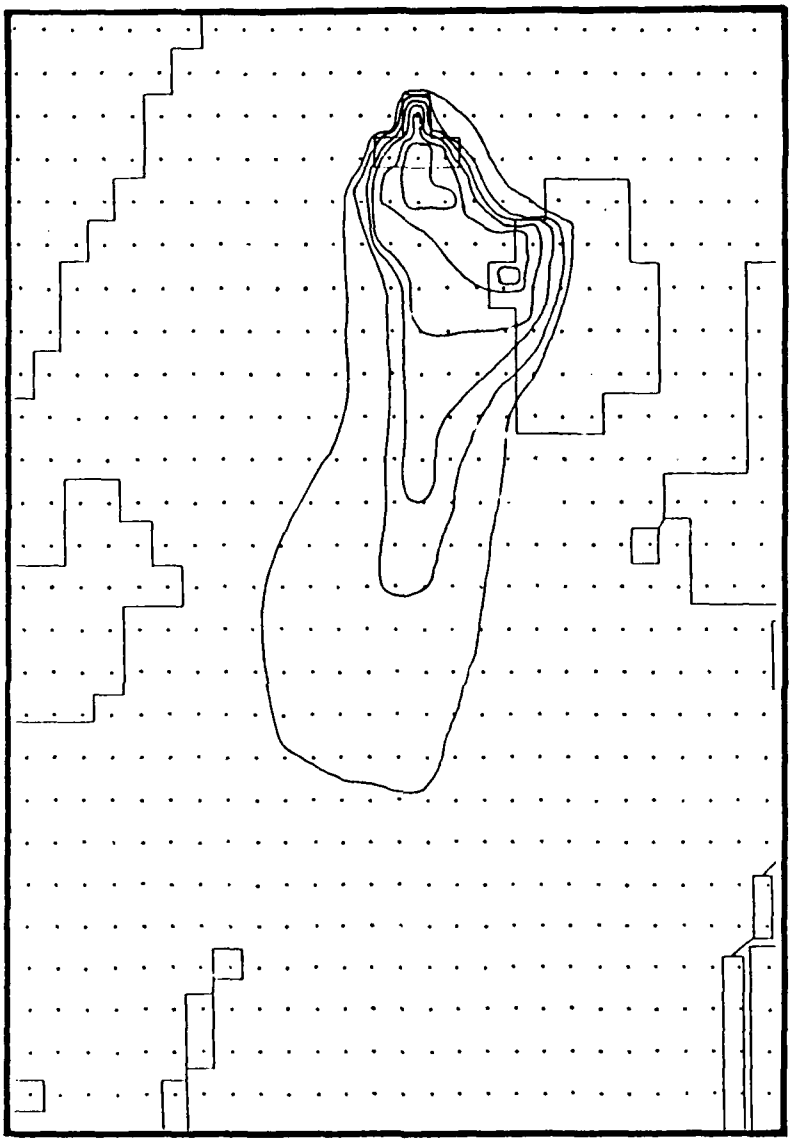

Figure 62. RW/Otis Plume Concentration Map for the Longitudinal Dispersion Coefficient Defined by DISPL = 40 Ft.

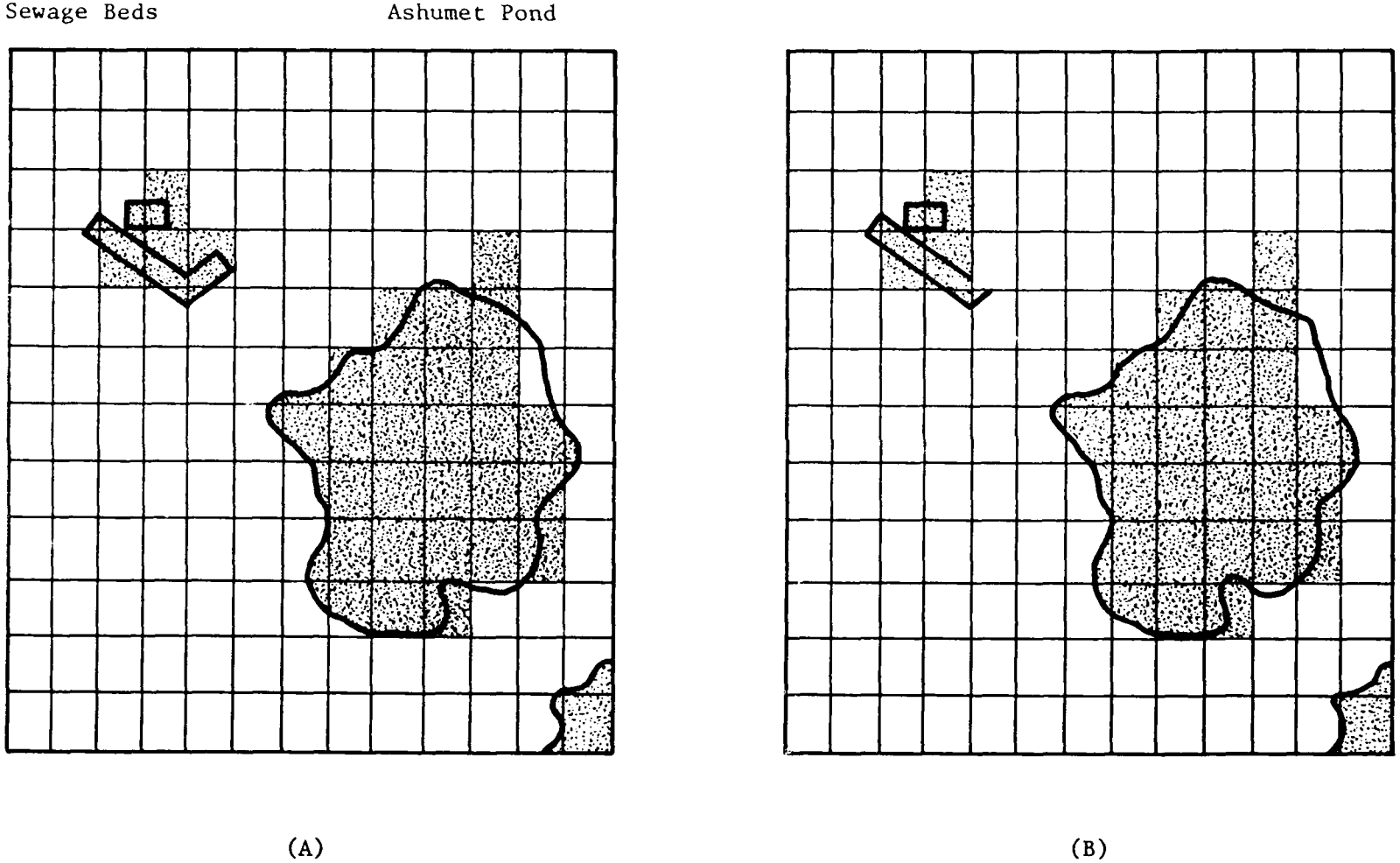

Figure 63. Revision of Sewage Bed Configuration: (A) Base Case, (B) Three Source-Cell Sewage Source.

63B. However, this did not significantly change either the shape of the plume, or its material balance.

The second change consisted of transforming cell (19,15) from a pond cell to a regular soil cell. As seen in Figure 64A, cell (19,15) protrudes from the pond's western shore. Based on previous results, we suspected this cell might have distorted the velocity field. However, a calibration run where cell (19,15) was changed from a pond cell to a normal soil cell showed no significant change.

Again with reference to the material balance, the aquifer's transmissivity values were considered. The input transmissivity values are only used for the first trial iteration. After that, transmissivity is recalculated cellwise each iteration as the product of hydraulic conductivity and saturated thickness. Saturated thickness is calculated each iteration using the updated valued of H(I,J). In the program, the MIN1 library function is used to determine if water table or artesian conditions are in effect, and to appropriately calculate saturated thickness. Hydraulic conductivity was specified as uniform over space and time. Therefore, transmissivity values can be further adjusted to account for any material imbalance.

As in the USGS-2D model, it was concluded that material imbalances are due to both models inadequately treating pollutant mixing within water bodies. That is, Ashumet Pond acts as a sink for solute coming from the sewage sand beds but the water source cells from the pond do not contribute solute to the aquifer.

The final calibrated pollutant plume is shown in Figure 65. This plume is used as the base case in the RW sensitivity studies. Appendix F lists the base case input data file for the Otis sewage plume for this modeling program.

C. SENSITIVITY STUDY

The results derived from the Random Walk sensitivity study are organized in terms of parameters with no effect, parameters with minimal effect, and parameters with appreciable sensitivity effects.

1. Parameters With No Effect

Several parameters in the RW model were eliminated from the sensitivity study, a priori, for the following reasons:

- Default card values were superceded by node card values, except for NC and NR.
- NSTEPS, NRT = 1 in all steady-state flow cases.
- X1, DX, Y1, DY, PL because subroutine GENP(PL) is effectively not used in Otis cases.
- T1(I,J), T2(I,J), and H(I,J) are initial trial values.

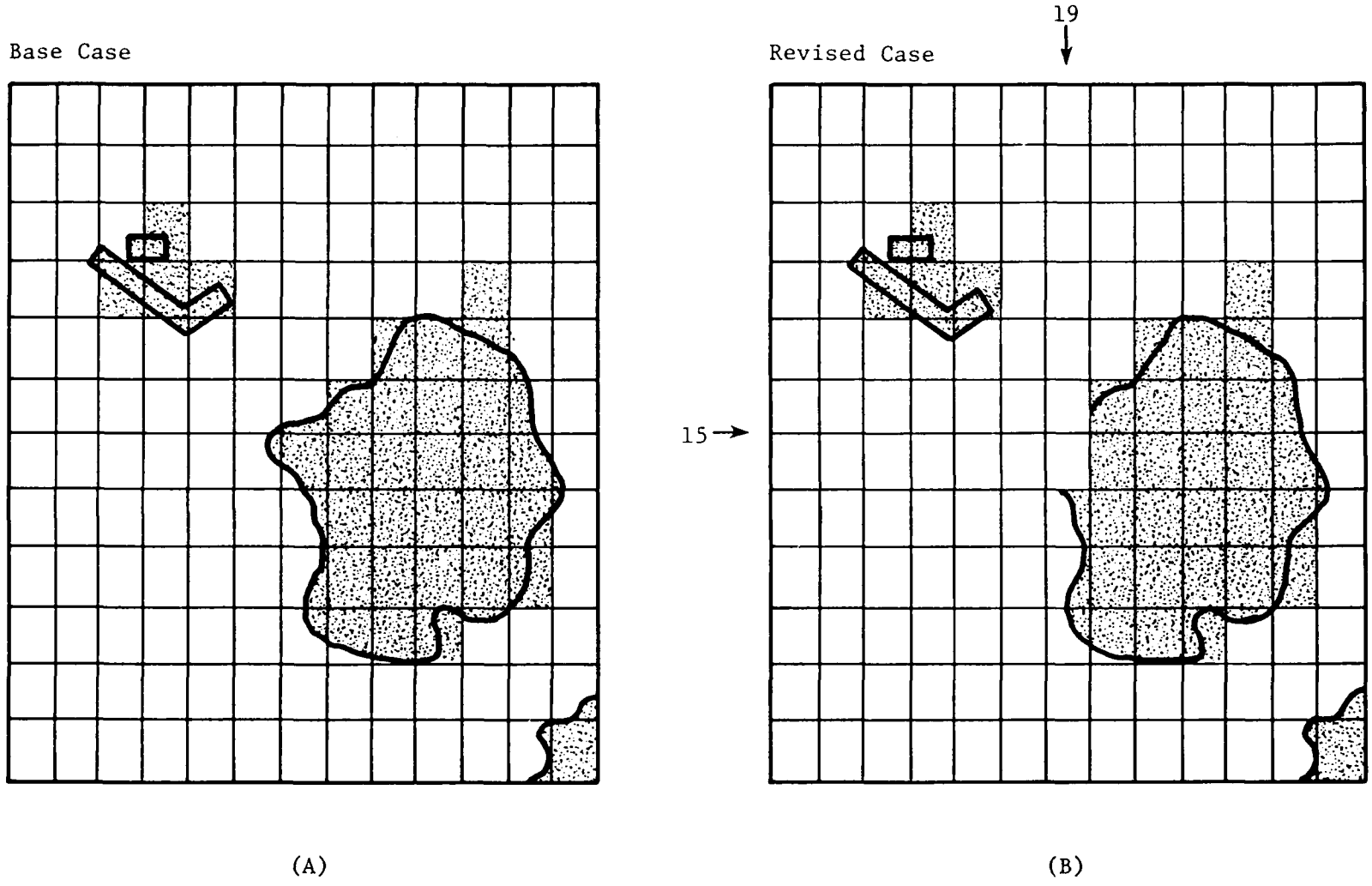

Figure 64. Revision of Ashumet Pond Configuration: (A) Base Case, (B) Replacing Pond Cell (19,15) by a Soil Cell (19,15).

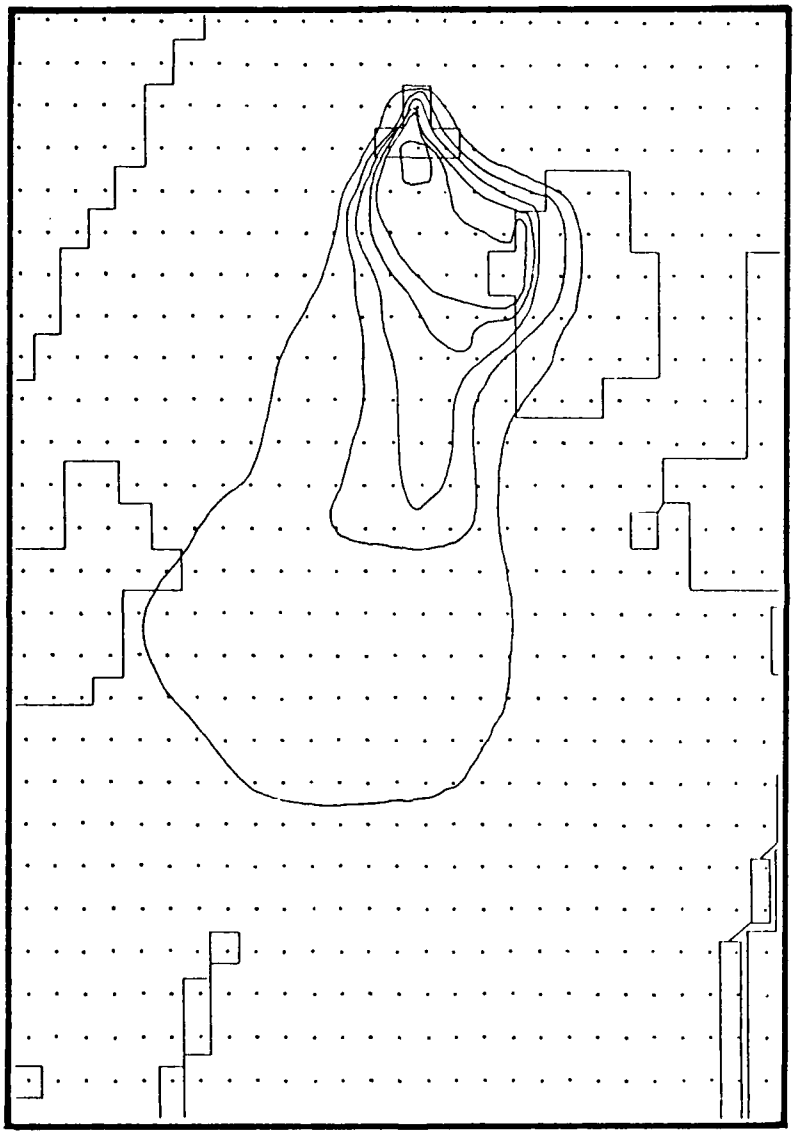

Figure 65. RW/Otis Plume Concentration Map for the Base Case, Run No. 2.

- NC, NR, DELX, DELY because finer discretization is not really necessary for the purposes of this study and would exceed the storage capacity available on the CYBER system.

- NPUMP, because no pumps are present.

- CH(I,J) has no effect on water table aquifers.

- BOTT(I,J) because the cell thicknesses vary between 90 to 140 feet so that adjustments within this range are not very important.

- RH(I,J), or the elevation of water surfaces, was found to vary by only ±1.5 feet between 1975 and 1984 (Reference 18).

- RD(I,J), or the elevation of the bottom of the pond's sediment layer, showed no visible sensitivity effects. Depth of Ashumet Pond was taken as 5 feet for edge cells and 10 feet for center cells.

The parameters that were tested are as follows:

ERROR	DELTA	NPITS
S2(I,J)	Q(I,J)	R(I,J)
pond depth	PERM1(I,J)	PERM2(I,J)
PM	DISPL	DISPT
APOR	EPOR	RD1
CPRD	DXMAX	DYMAX
NSP	S1(I,J)	

A complete list of the sensitivity runs made in this study is given in Table 11. From these runs, two more parameters were found to have no affect on the simulated results. They are:

- NSP, or the number of time increments per pumpage period. NSP > 1 is likely to improve accuracy and speed of convergence for unsteady-state flow cases, but is unlikely to affect solutions for steady-state cases. Reference 6 uses NSP = 2 for its steady-state flow sample problems. In our sensitivity analyses, NSP = 1,2, and 4 gave essentially the same results. Presumably, either 1 or 2 is acceptable.

- S1(I,J), or the storativity under artesian conditions. This quantity has no effect under steady-state flow conditions because water table levels and pressures remain constant.

2. Parameters With Minimal Effects

In the Random Walk model, weak variations due to parametric sensitivity tests may not be discernable from the inherent variabilities produced by the random component of the model. For example, Figures 65 to 67 show three distinct base case runs for the RW model. Each time the base case input file is run, the output data will be slightly different because of the random number generator used in the code. Thus, any parameter which realistically has a small operating range about some mean value, or base case value, may produce an output variability which may be masked by the inherent

TABLE 11. LIST OF RANDOM WALK SENSITIVITY RUNS.

PARAMETERS (UNITS)	PARAMETERS (UNITS)
DISPL = 125 ft.	SO. CONC = 1. ppm (drafting template)
DISPL = 125 ft. (repeated)	
DISPL = 100 ft.	SO. CONC = 400. ppb,
DISPL = 150 ft.	SO. CONC = 600. ppb
DISPL = 150 ft. (repeated)	
DISPL = 175 ft.	RD = 1.25
DISPL = 200 ft.	RD = 3.0
DISPL = 300 ft.	
DISPL = 40 ft.	DXMAX = 0.150
DISPL = 0.10 ft.	DXMAX = 0.100
DISPL = 75 ft.	DXMAX = 0.075
DISPL = 125 ft. (repeated)	DXMAX = 0.050
DISPL = 500 ft.	
	S1 = 1.0E-5
CPRD = 0.400	S = 1.0E-3
CPRD = 0.450	
CPRD = 0.500	Q = 10.13E3
CPRD = 0.525	Q = 15.20E3
CPRD = 0.550	
	RECH(B) = 32.3 RECH(C) = 0.646
NSP = 1	RECH(B) = 129.3 RECH(C) = 2.586
NSP = 2	
NSP = 4	POND DEPTH = 2.5 ft(B) = 5.0 ft(C)
DELTA = 14610. days	POND DEPTH =10.0 ft(B) = 10.0ft(C)
DELTA = 365.25 days	
DELTA = 30.4 days	SF2 = 0.28
	SF2 = 0.42
ERROR = 1.00 ft.	
ERROR = 10.00 ft.	PERM = 1120 Gal/day-sq.ft.
ERROR = 100.00 ft.	PERM = 1680 Gal/day-sq.ft.
PM = 3545 lb.	
PM = 6000 lb.	
PM = 6000 lb. (repeated)	PM = 1000 lb. NPMAX = 9000
NPITS = 20 DELP = 730.5 days	SF2 = 0.420 PM = 1000 lb.
NPITS = 80 DELP = 365.3 days	
	DXMAX = 0.200 DELP = 365.25
RD = 1.50	DXMAX = 0.200 DELP = 182.63
RD = 2.00	DXMAX = 0.100 DELP = 365.25
	DXMAX = 0.100 DELP = 182.63
APOR = 0.30 EPOR = 0.30	
APOR = 0.35 EPOR = 0.30	
DISPT = 12.5 ft.	
DISPT = 125.0 ft.	

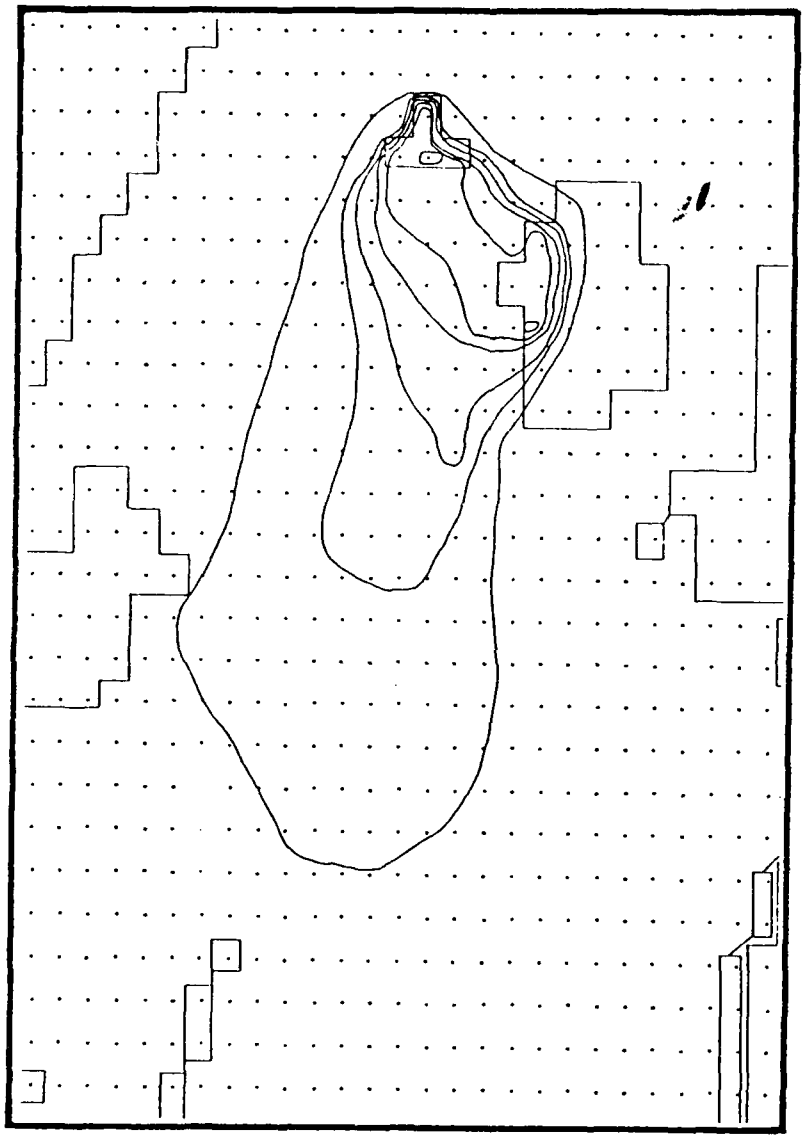

Figure 66. RW/Otis Plume Concentration Map for the Base Case, Run No. 1.

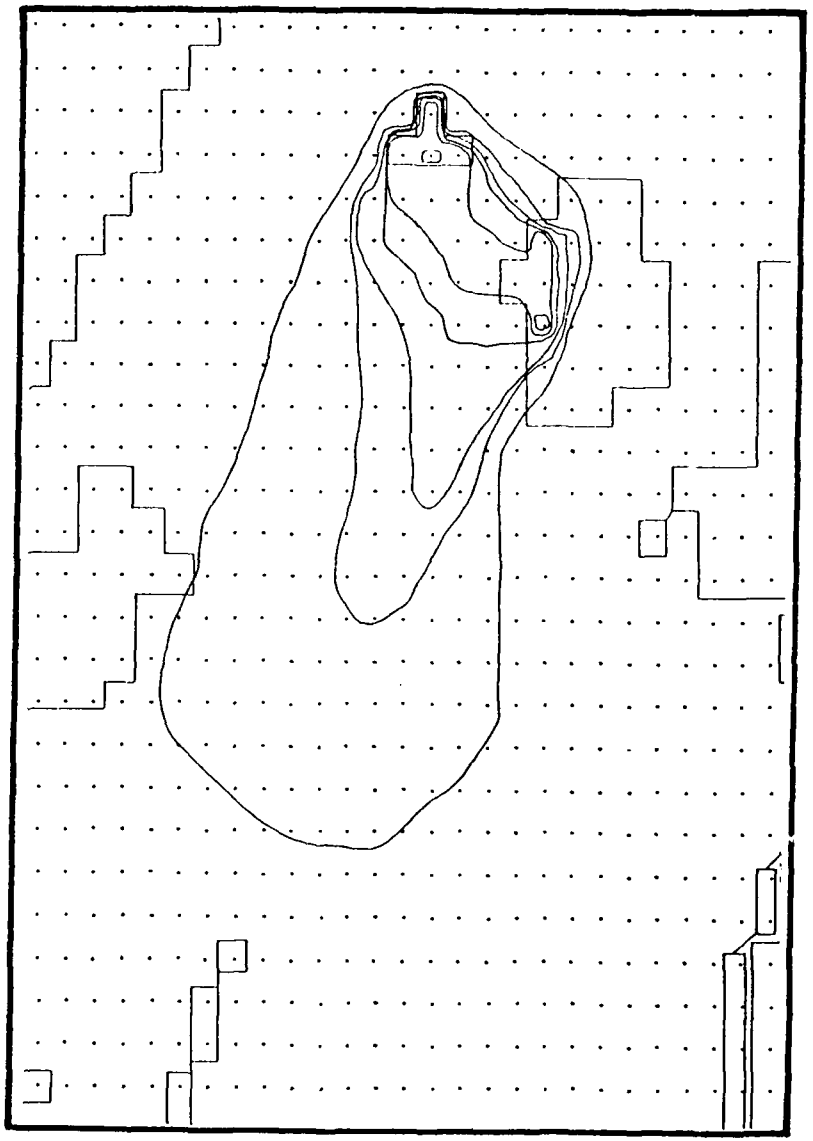

Figure 67. RW/Otis Plume Concentration Map for the Base Case, Run No. 3.

variability of the random component of the model, as exhibited by the variations between Figures 65, 66, and 67.

Parameters found to be in this category of "minimal effects" are discussed in the following subsections.

a. Ashumet Pond Leakance Coefficients

The leakance coefficients for the cells covering Ashumet Pond have to be large enough to maintain the proper water levels and to produce the observed pollutant plume shape. In this study, the base case values of R(I,J) = 64.6 gal/day-ft along the pond's shore and R(I,J) = 1.29 gal/day-ft in the pond's interior were used. Larger values will result in constant head nodes. These values had no visible effects in the USGS-2D and RW simulations. However, if these leakance coefficients are reduced by 90 percent or more, changes in the plume map will be visible. A similar effect, a 97 percent reduction in leakance coefficients in a USGS-2D simulation, is shown in Figure 38 (compare with Figure 37).

b. DELTA

DELTA is the duration of the time increments in the RW model's head solver. DELTA is taken to be 1.0E10 days. DELTA must be large, but need not be any particular value. Reducing DELTA from 1.0E10 to 1.46E4 had very little effect. But further large reductions had an effect, as shown in Figures 68 and 69.

c. NPITS and DELP

DELP is the duration of the time increments used in the movement of particles. While (NPITS)(DELP) must equal the time period simulated, 40 years in this case, the particular pair of (NPITS)(DELP) values was unimportant. No significant effect was seen in the plume concentration maps for the sensitivity runs listed in Table 11. Increasing NPITS increased the frequency of the solute transport printouts, while DELP changes had little effect on the frequency of recalculation of particle trajectories (usually DXMAX and DYMAX are more important than DELP in this respect).

d. ERROR

ERROR is the head solver convergence tolerance in feet. The steady-state default value of ERROR = 0.10 feet was used in this study. The iterative process in the head solver is stopped when the sum of the head changes over all nodes produced by one time increment is less than or equal to ERROR.

Setting ERROR > 1 foot has a visible effect on the simulated plume; ERROR > 10 feet has an even stronger effect. The effects of varying ERROR can be seen in Figures 70 and 71, the plume maps for ERROR = 10 and ERROR = 100, respectively.

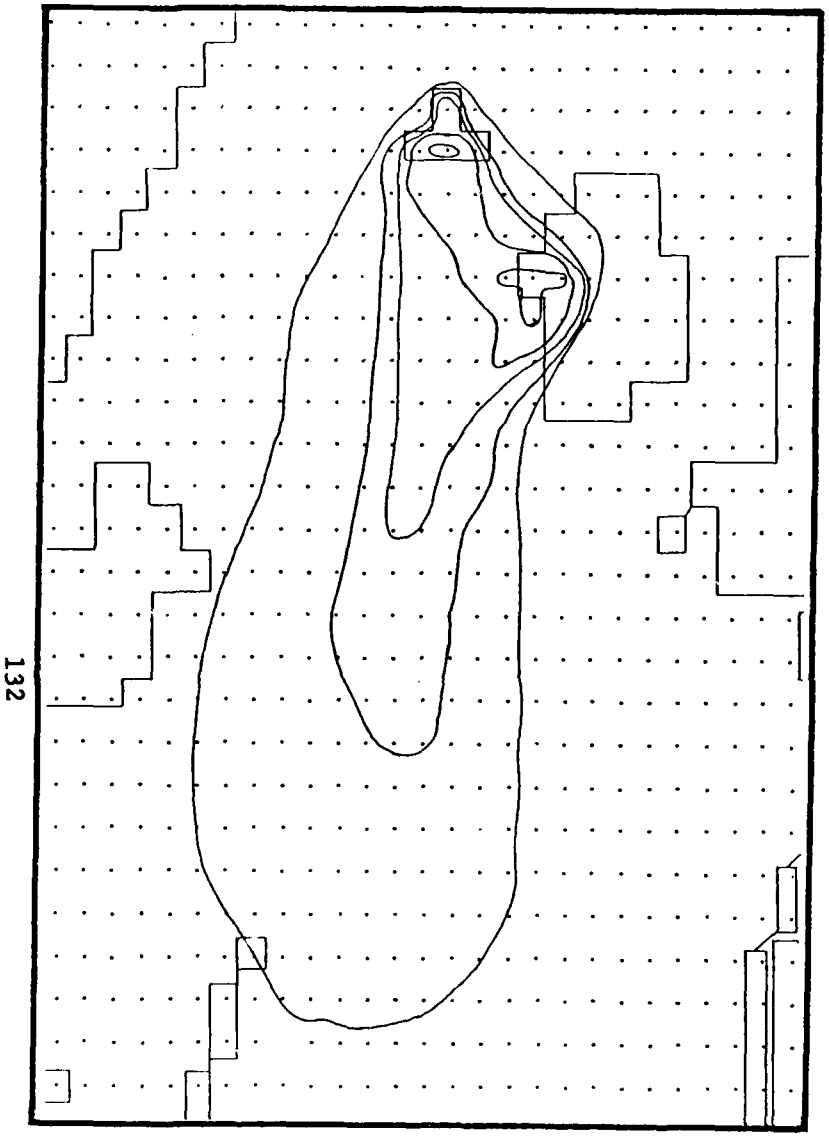

Figure 68. RW/Otis Plume Concentration Map for DELTA = 365.3 Days.

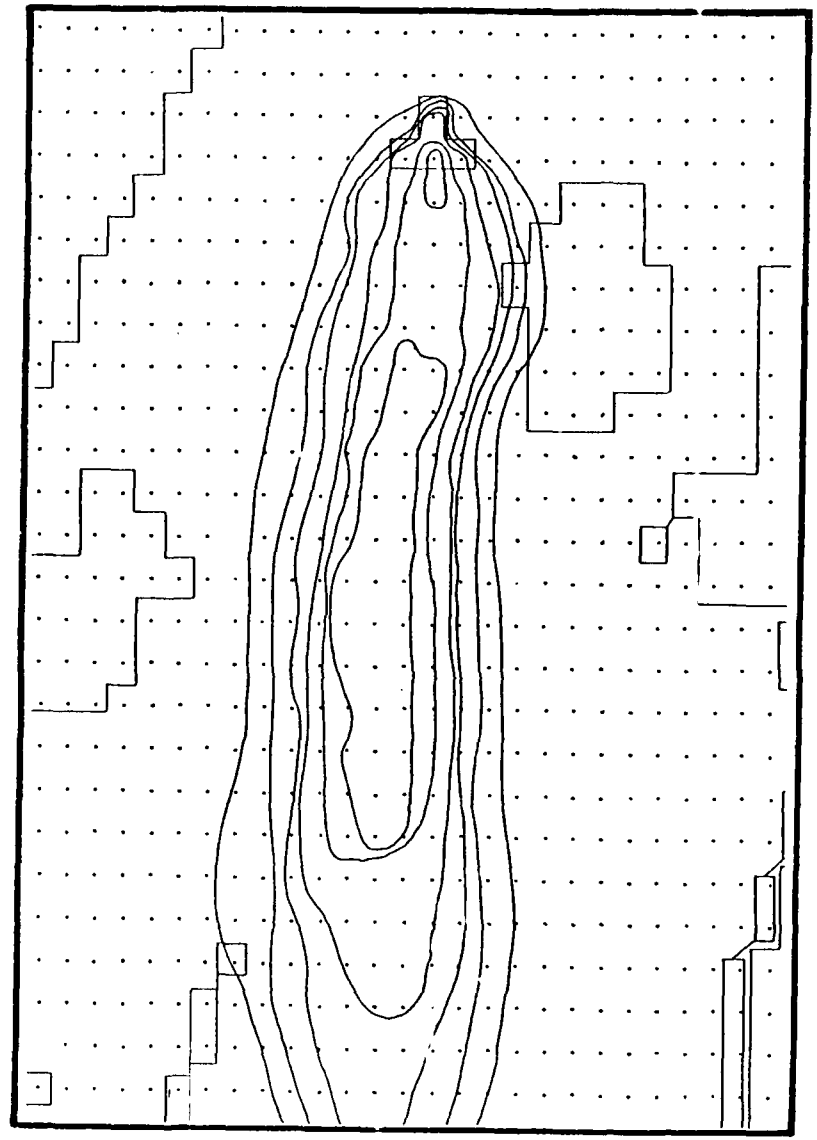

Figure 69. RW/Otis Plume Concentration Map for DELTA = 30.4 Days.

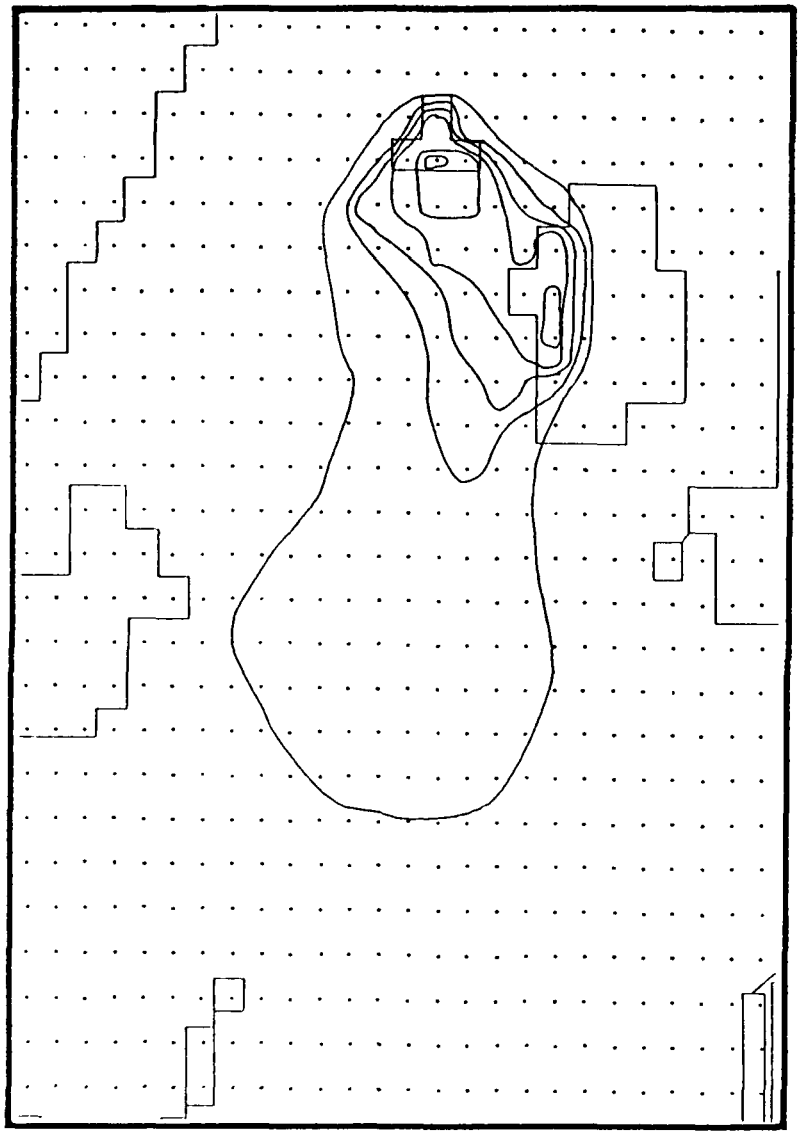

Figure 70. RW/Otis Plume Concentration Map for ERROR = 10.

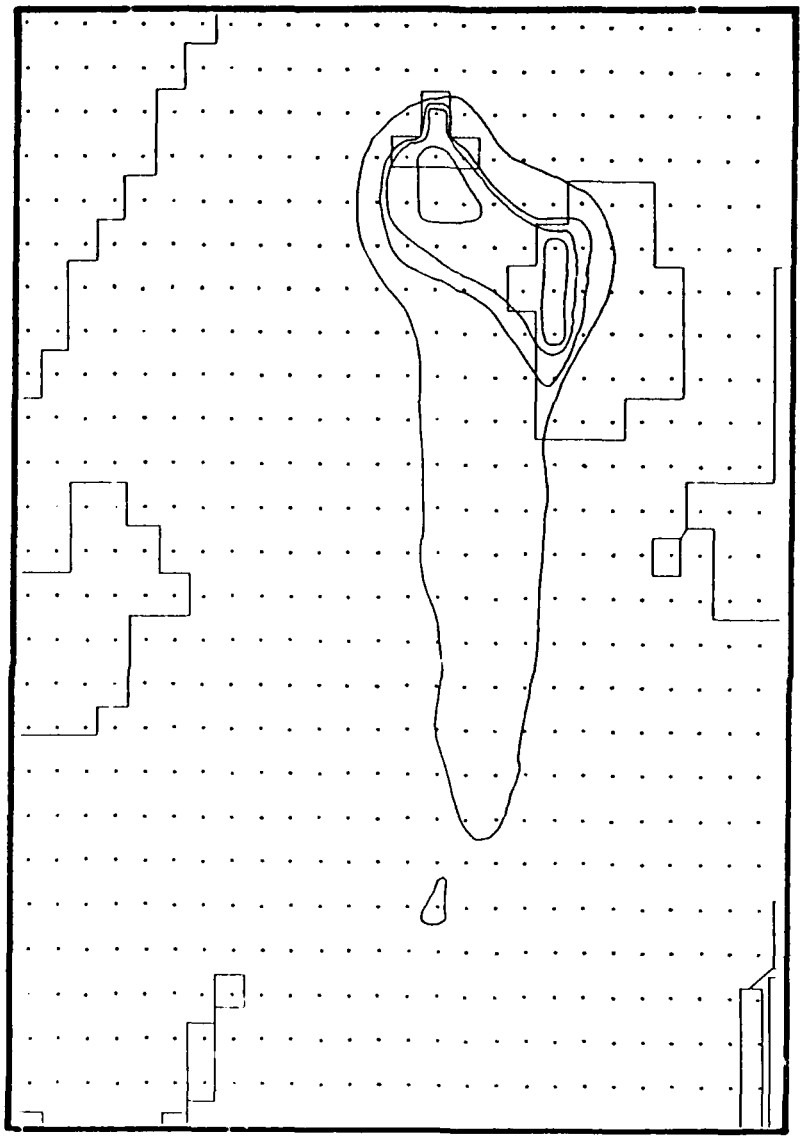

Figure 71. RW/Otis Plume Concentration Map for ERROR = 100.

e. MAXP

MAXP is the maximum number of solute particles allowed in the model aquifer during any given time. When MAXP = 9000, our study requires PM to equal 1750 pounds of pure solute per particle. Approximately 17,500 particles enter the aquifer over 40 years, but about half of these are gradually lost through the Ashumet Pond sinks.

Acceptable simulations were run with fewer than 9000 particles, but the use of 9000 gives smoother, more easily readable plume maps. This value of MAXP is required for the southern end of the plume to be smooth, where there are usually only 1 to 4 particles per cell. The CYBER system's limitations on core memory per user prevent the use of substantially more particles per run.

f. DISPT

DISPT is the transverse dispersivity in feet. Generally, DISPT = (0.1 to 0.5) (DISPL). The effects of varying DISPT is shown in Figures 72 and 73. However, as was the case at Otis, the value of DISPT is usually taken as DISPT ≅ (0.3) (DISPL).

g. DXMAX and DYMAX

DXMAX and DYMAX are the components of the maximum travel distance between particle-velocity reinterpolations. The units of these quantities are given in fractions of cell length and width. In the base case, DXMAX = DYMAX = 0.20. Sensitivity runs were made at DXMAX = DYMAX = 0.05, 0.10, 0.15, without noticeable changes in the plume map outputs. In the base case, most particles will have a velocity calculated once per DELP period. It is usually more efficient to reduce DXMAX and DYMAX than DELP, as discussed in Appendix E.

3. Parameters With Appreciable Effects

Six parameters were found to appreciably affect the pollutant plume during the sensitivity study. Their effects are discussed in the following subsections.

a. Aquifer Porosities

S2(I,J) is the storativity for water table aquifer conditions. This parameter is used in the head solver routine and is related to the fractional volumetric porosity. APOR is the actual porosity, which is used in the solute transport routine. EPOR is the fractional effective porosity used in the solute transport routine to account for tortuosity and dead end pore effects. As APOR decreases, the pollutant plume tends to spread out (compare Figures 74 and 75).

b. Hydraulic Conductivity

PERM1(I,J) and PERM2(I,J) are measures of the hydraulic conductivities in the x- and y-directions, respectively. These values are entered cell-by-cell in the "node card" lines. Unlike transmissivity values,

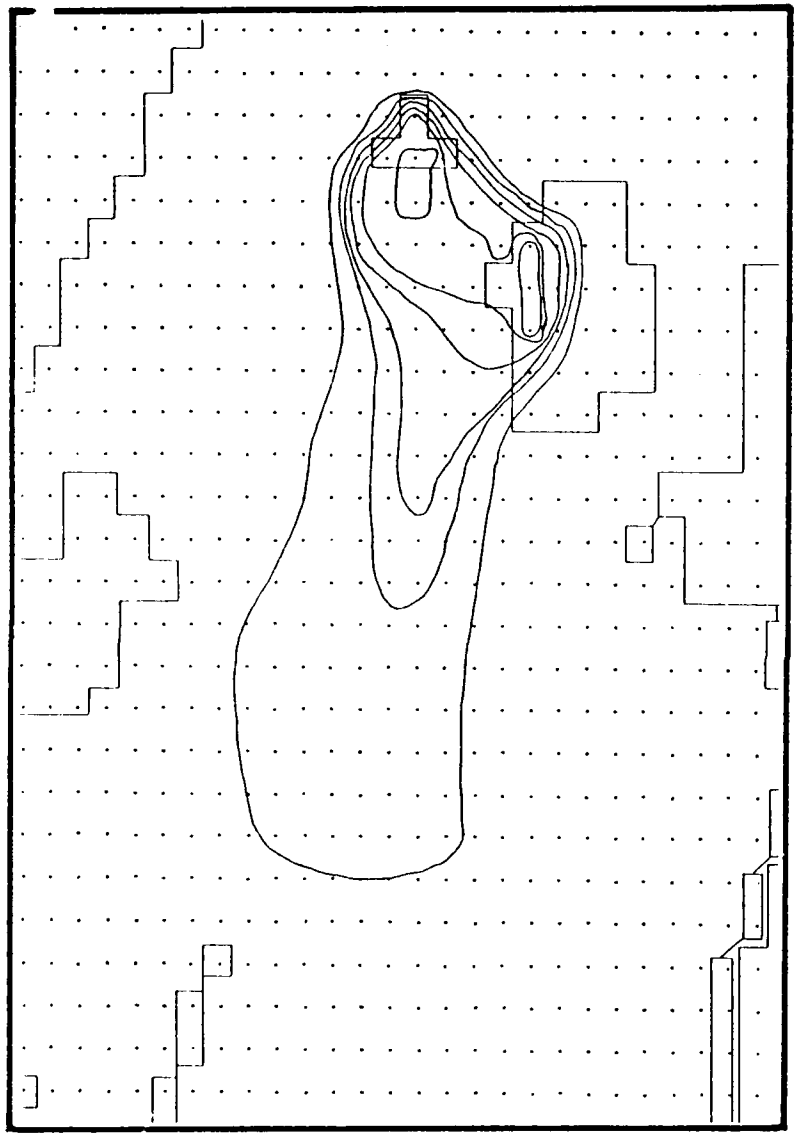

Figure 72. RW/Otis Plume Concentration Map for DISPT = 12.5 Ft.

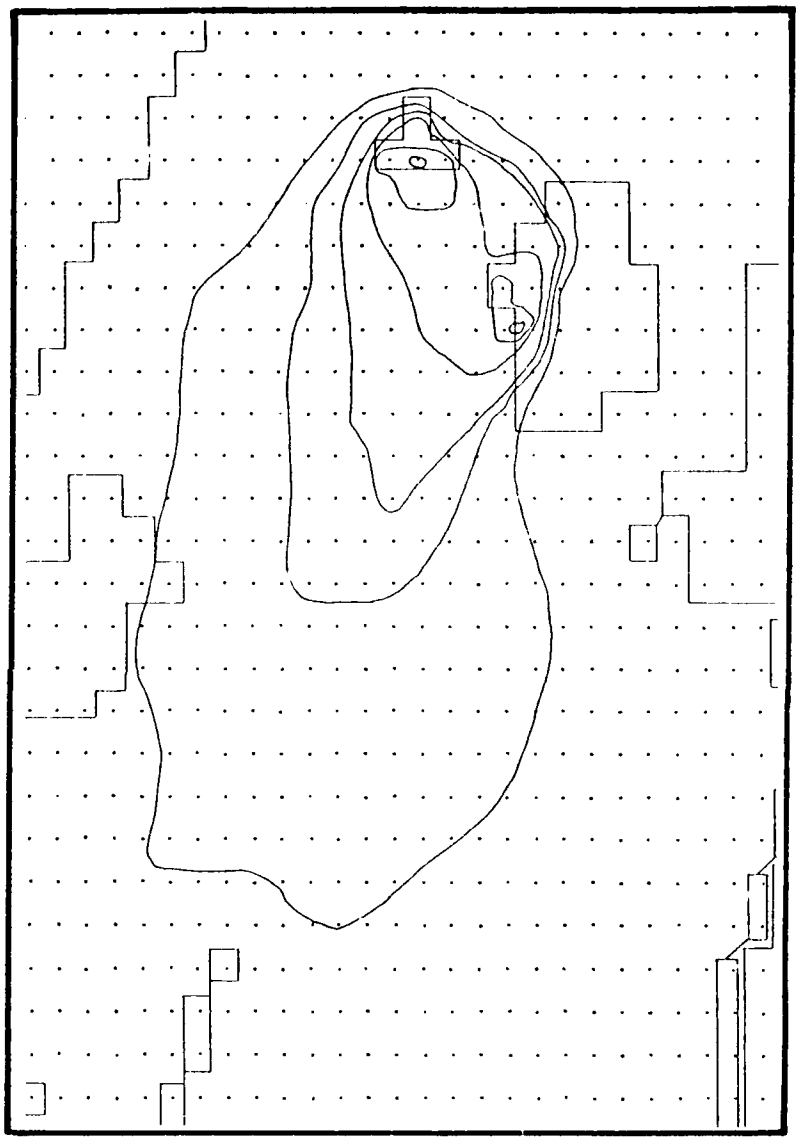

Figure 73. RW/Otis Plume Concentration Map for DISPT = 125 Ft.

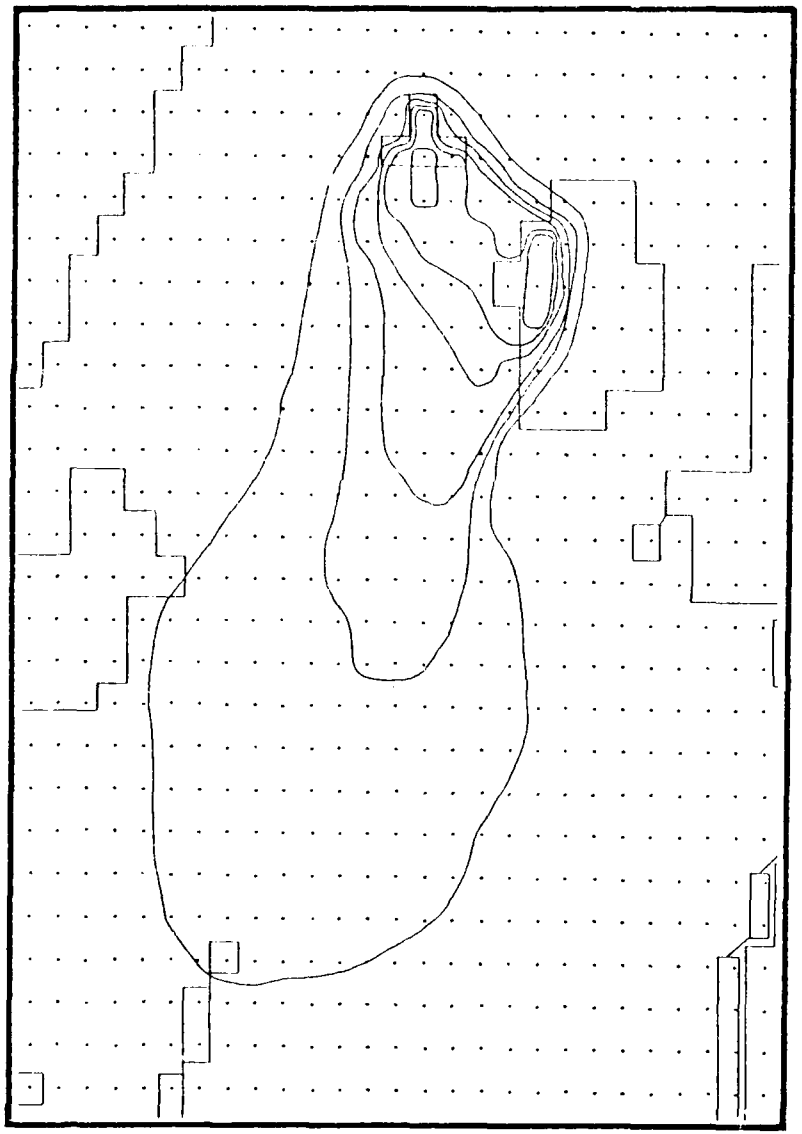

Figure 74. RW/Otis Plume Concentration Map for APOR = 0.30 and EPOR = 0.30.

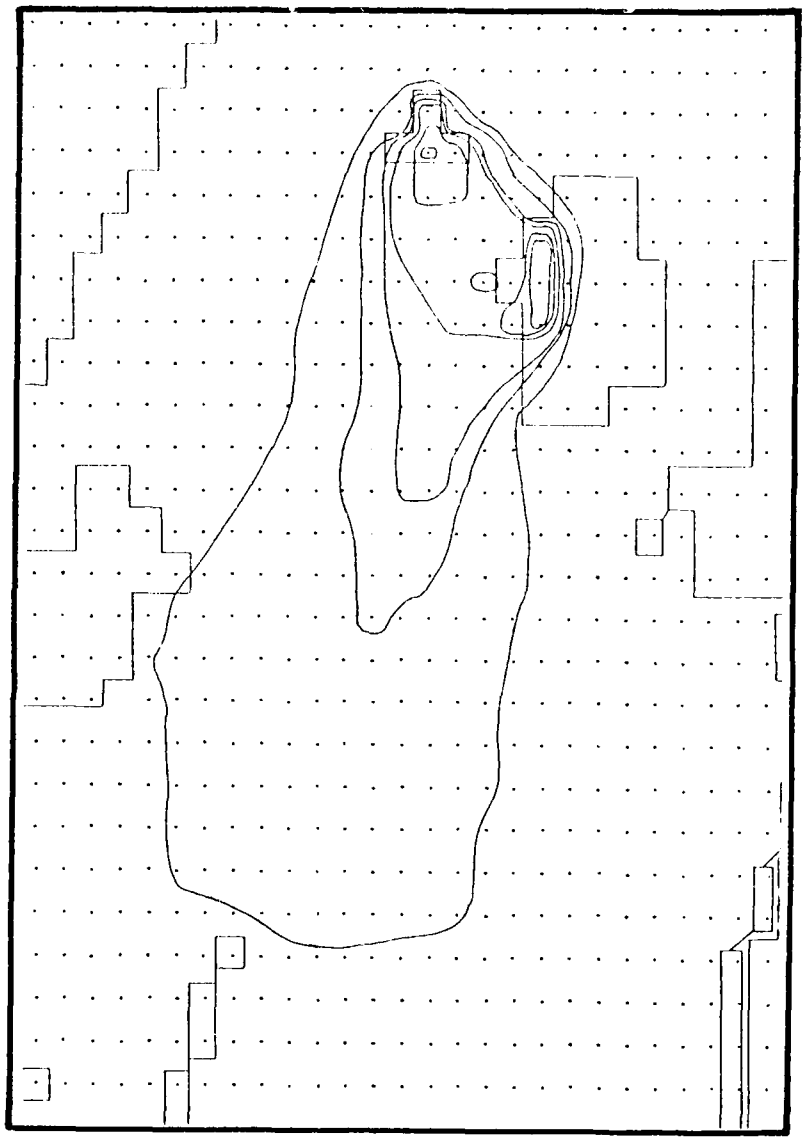

Figure 75. RW/Otis Plume Concentration Map for APOR = 0.35 and EPOR = 0.30.

which are only initial trial values, permeability values significantly affect the concentration plume maps. Increased hydraulic conductivity values decrease the hydraulic gradients, causing the plume to spread out and to have lower concentrations near the sand beds. Two such plume maps are shown in Figures 76 and 77.

c. Nodewise Leakance Rates

Q1(I,J) are leakance rates, specified by node, as distributed flows in the area surrounding each node. Rainfall recharge was specified for all nodes except those under the ponds. Additional flows were specified for sewage sources at the sand beds, and for groundwater inflow at the northern boundary. Evapotranspiration was neglected at Otis, but could be significant in semi-arid locations.

Concentration plume maps for these sensitivity runs are shown in Figures 78 and 79. A 20 percent decrease in the average rainfall recharge rate (Figure 78) noticeably expanded the lower concentration contours, and shrank the highest concentration contours. A 20 percent increase in the rainfall recharge rate (Figure 79) had the opposite effects because more solute is flushed out through the Ashumet Pond sinks.

d. Longitudinal Dispersivity

DISPL is the longitudinal dispersivity in feet, and was discussed under the subsection on "Calibration." The base case value of DISPL is 125 feet (Figures 65, 66, and 67). A plume map for DISPL = 40 feet is shown in Figure 62. Additional plume maps for varying DISPL are shown in Figures 80 (0.1 feet), 81 (75 feet), 82 (175 feet), 83 (300 feet), and 84 (500 feet.).

e. Source Concentration

CONSOR(I,J) is the solute source concentration which is specified in the node data lines. Four source cells were specified, representing the sewage plant effluent at the sand beds. In the base case, the source concentration of the rain water plus sewage was set at 500 ppb. In sensitivity runs, this concentration was changed to 600 ppb and 400 ppb, as shown in Figures 85 and 86, respectively. As expected, the solute concentrations within the plume varied proportionally, and the concentration contour lines expanded or contracted accordingly.

f. Retardation Factor

RD1 is the retardation factor given by RD1 = 1.0 + (KD)(DENS)(EPOR) = $\frac{v}{v_c}$, where v_c = velocity of the concentration front. RD1 = 1.0 for nonadsorption cases, while RD1 > 1.0 for adsorption cases.

Four sensitivity runs were made for RD1 > 1. Figures 87 through 90 show the results of these runs for the values of RD1 = 1.25, 1.50, 2.00, and 3.00, respectively.

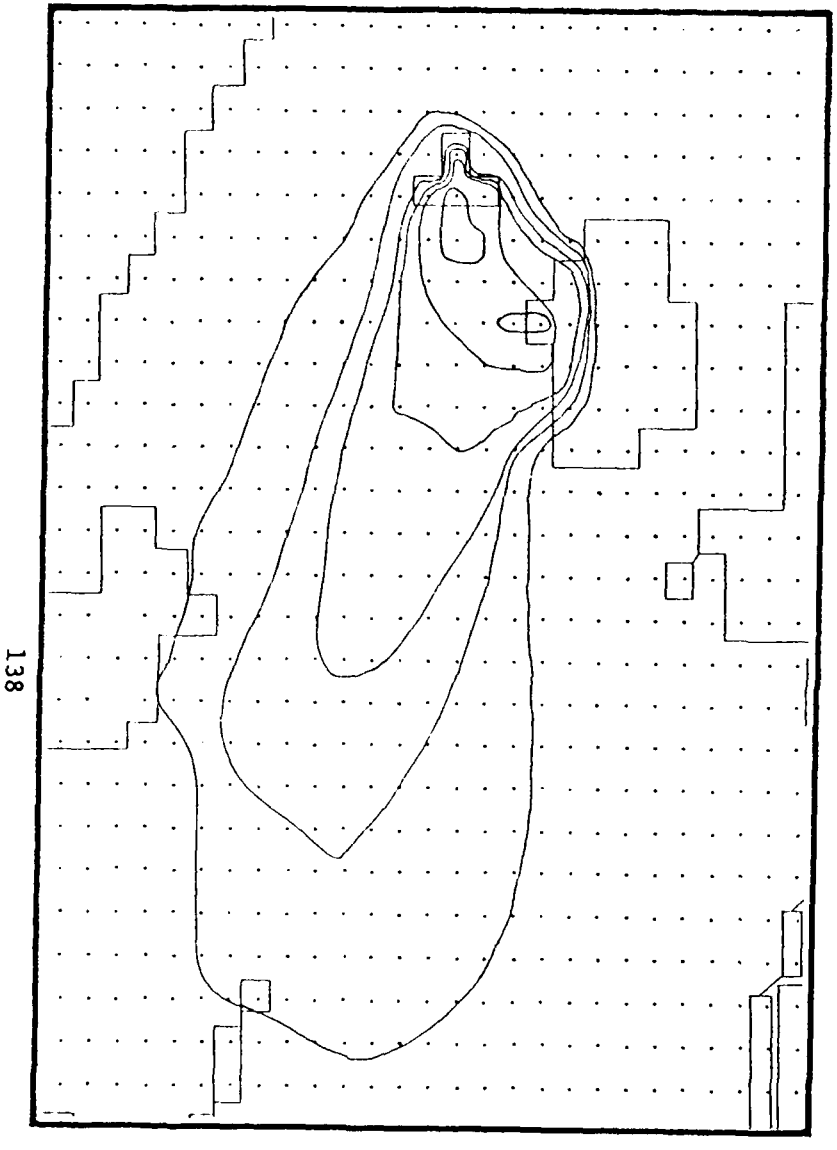

Figure 76. RW/Otis Plume Concentration Map for PERM = 1680 gal/day-sq. ft.

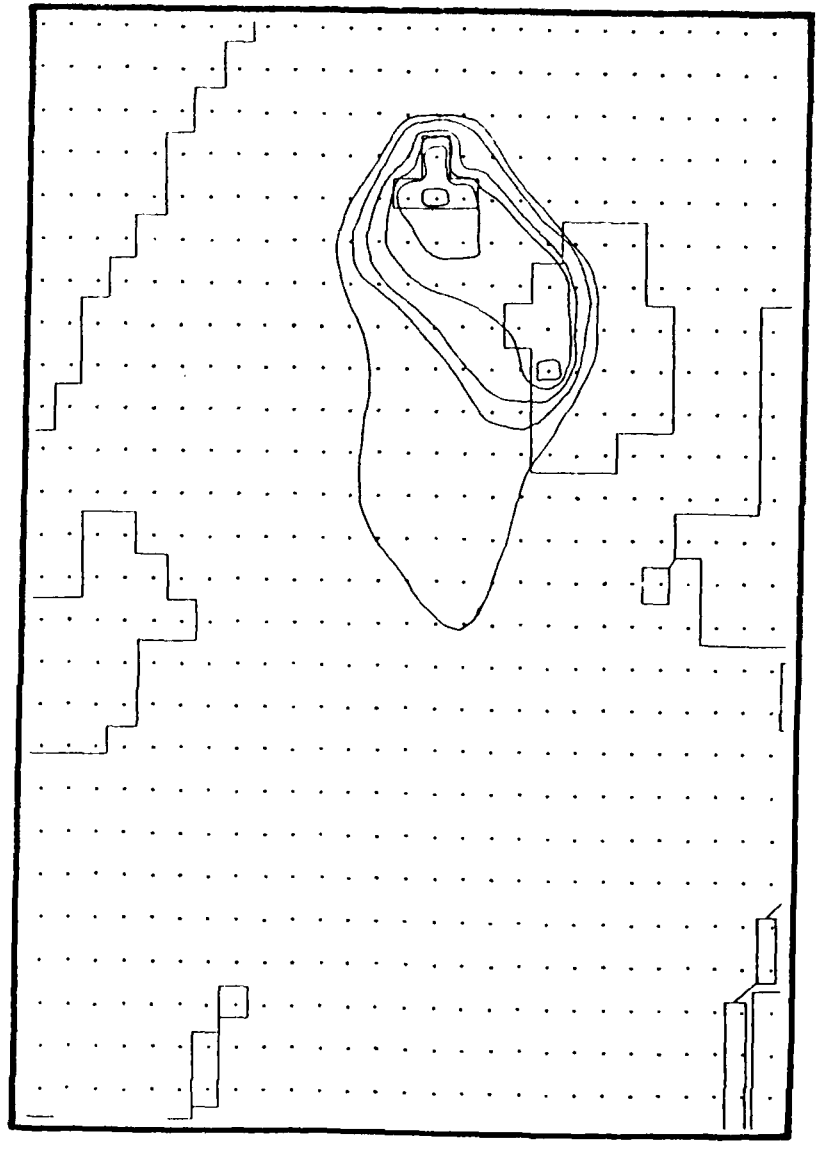

Figure 77. RW/Otis Plume Concentration Map for PERM = 1120 gal/day-sq. ft.

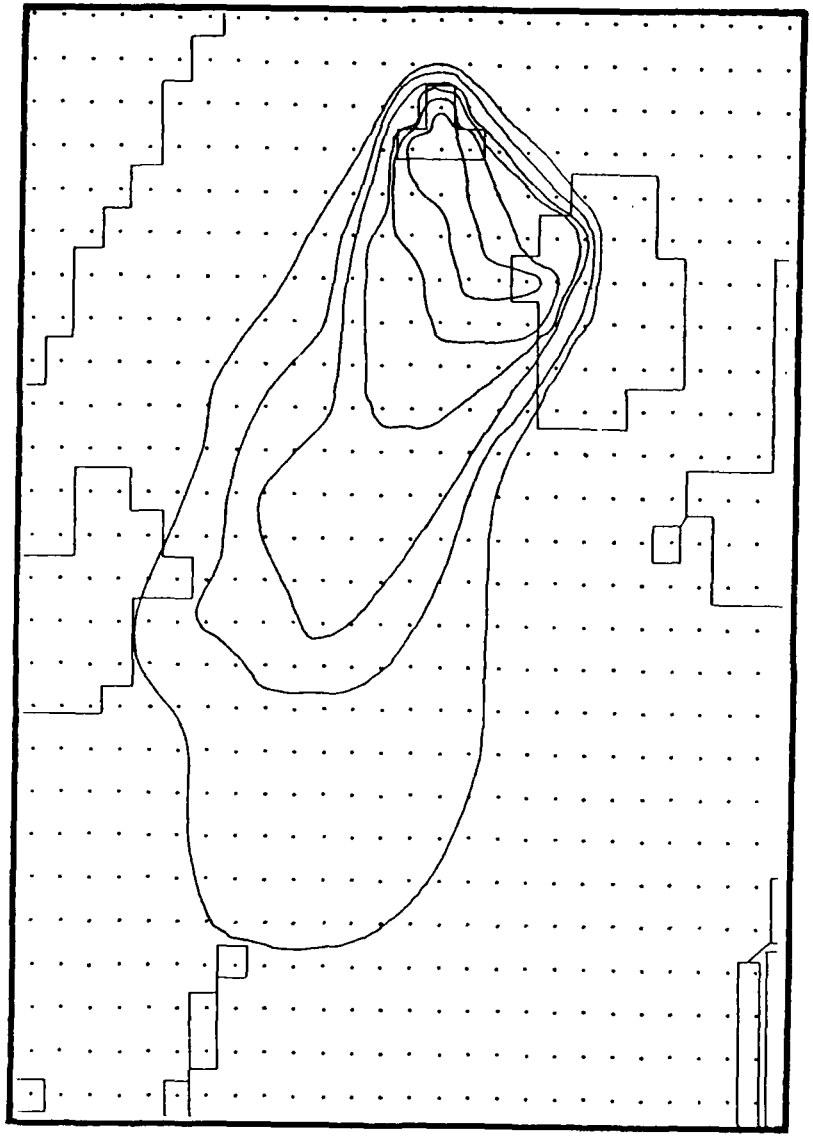

Figure 78. RW/Otis Plume Concentration Map for Q = 10.13E3.

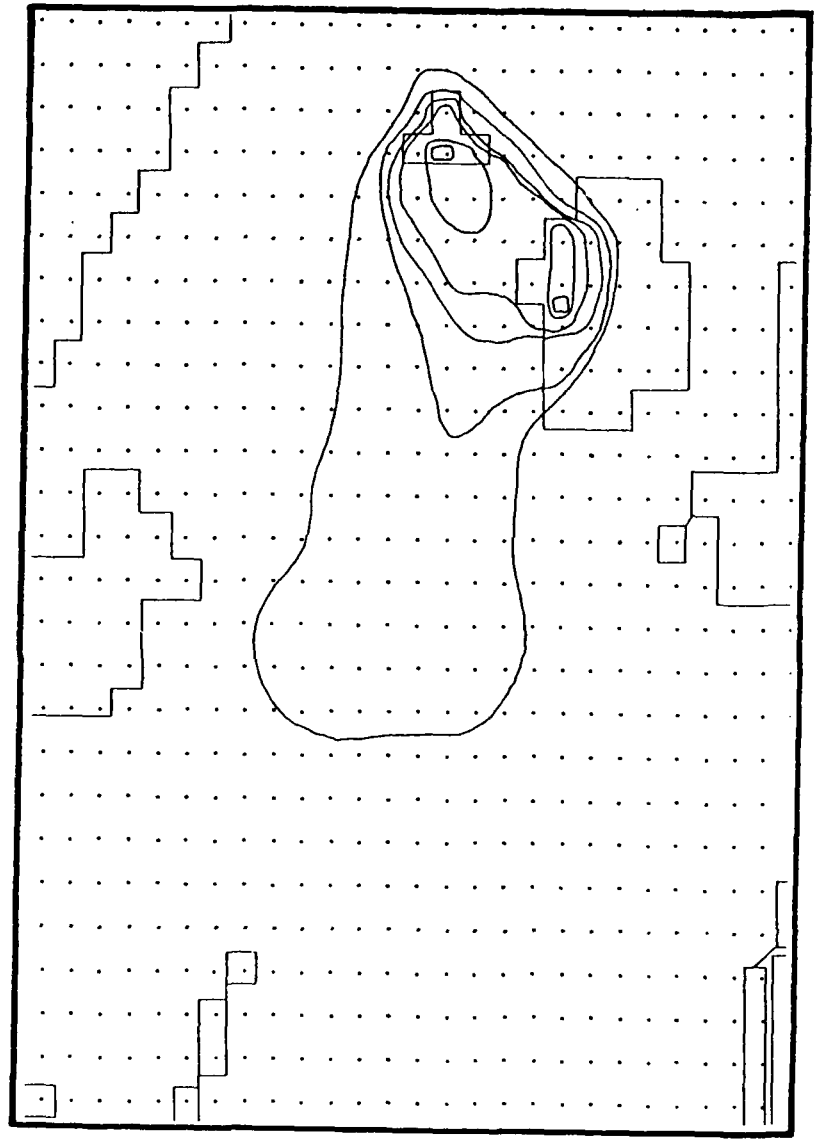

Figure 79. RW/Otis Plume Concentration Map for Q = 15.20E3.

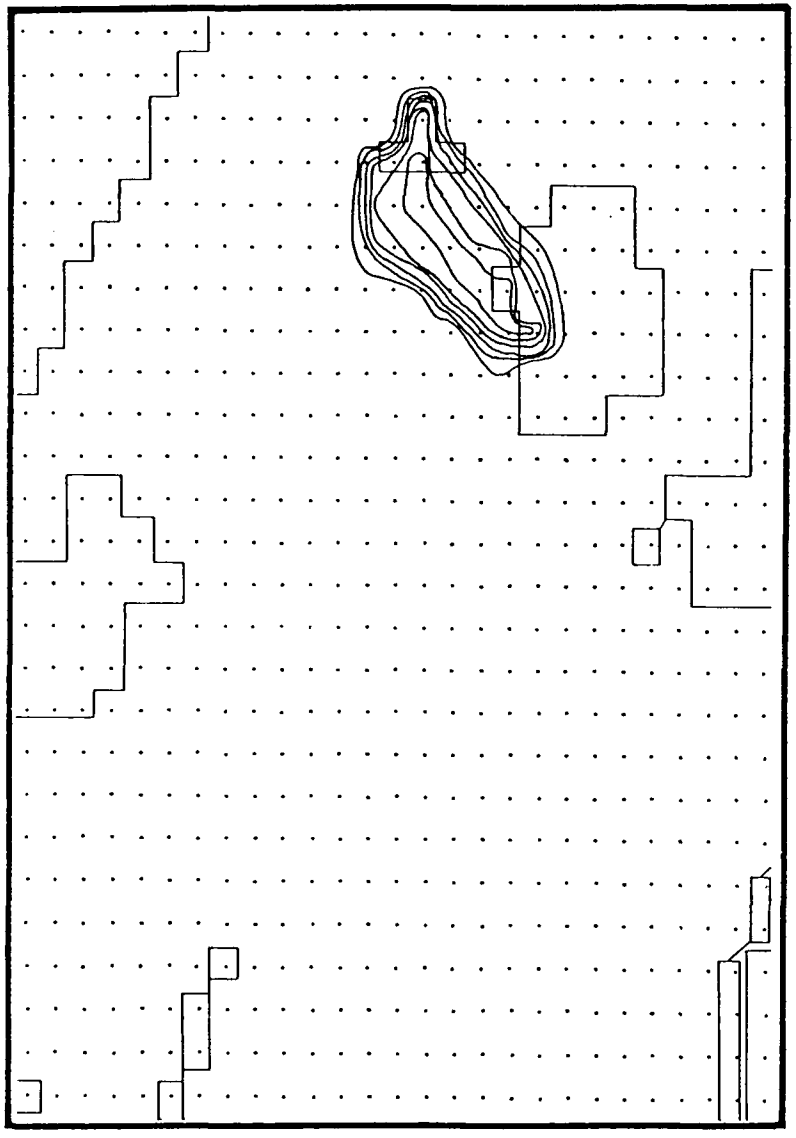

Figure 80. RW/Otis Plume Concentration Map for DISPL = 0.1 Ft.

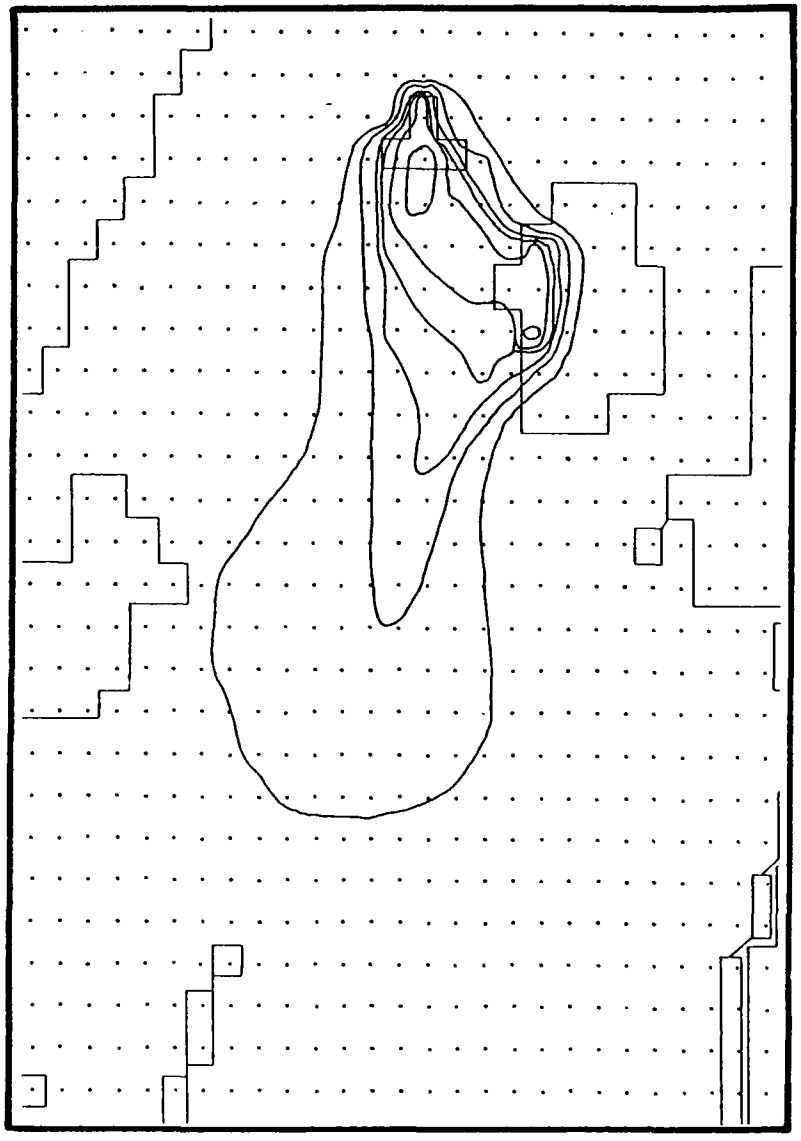

Figure 81. RW/Otis Plume Concentration Map for DISPL = 75 Ft.

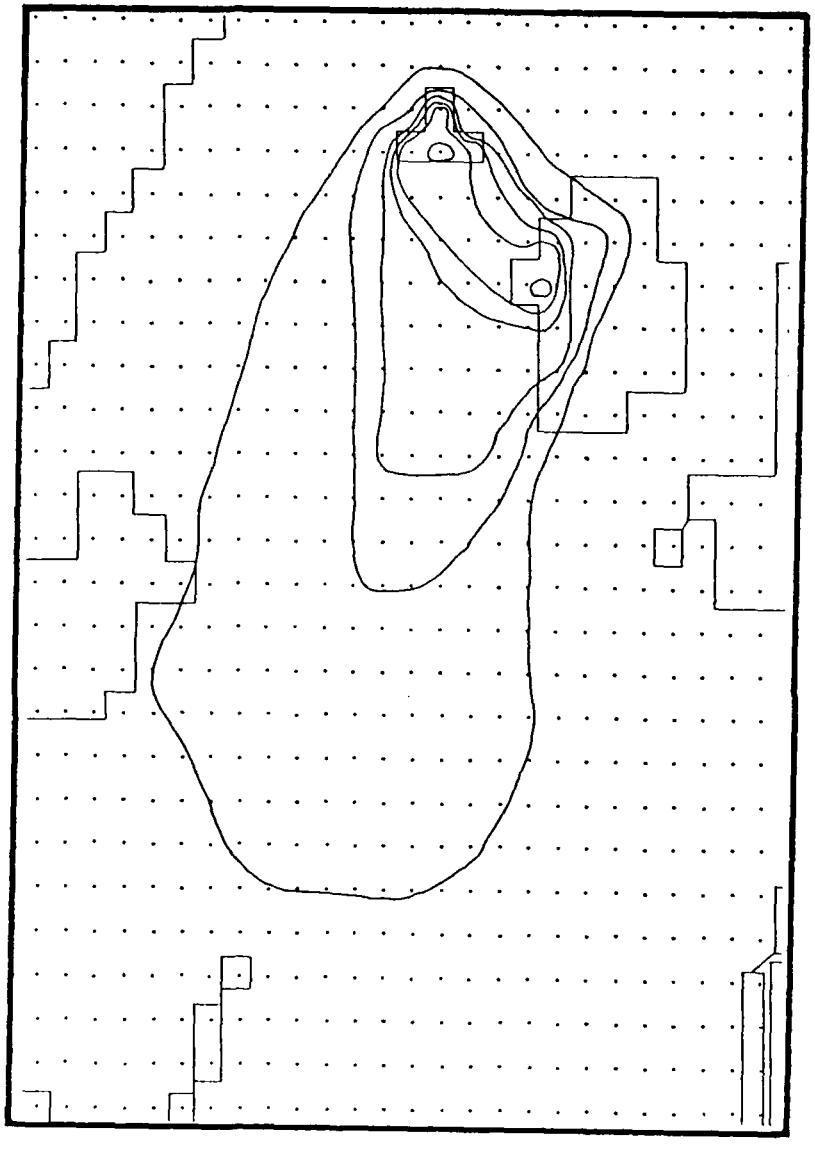

Figure 82. RW/Otis Plume Concentration Map for DISPL = 175 Ft.

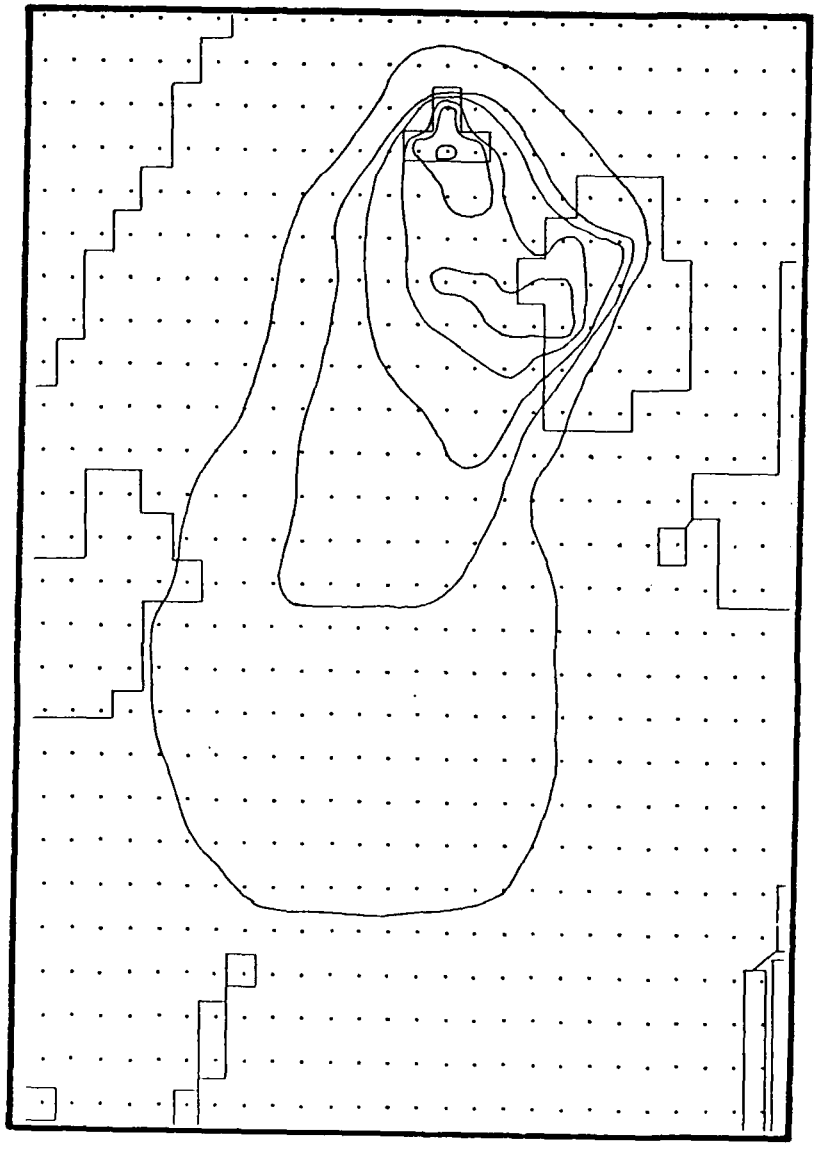

Figure 83. RW/Otis Plume Concentration Map for DISPL = 300 Ft.

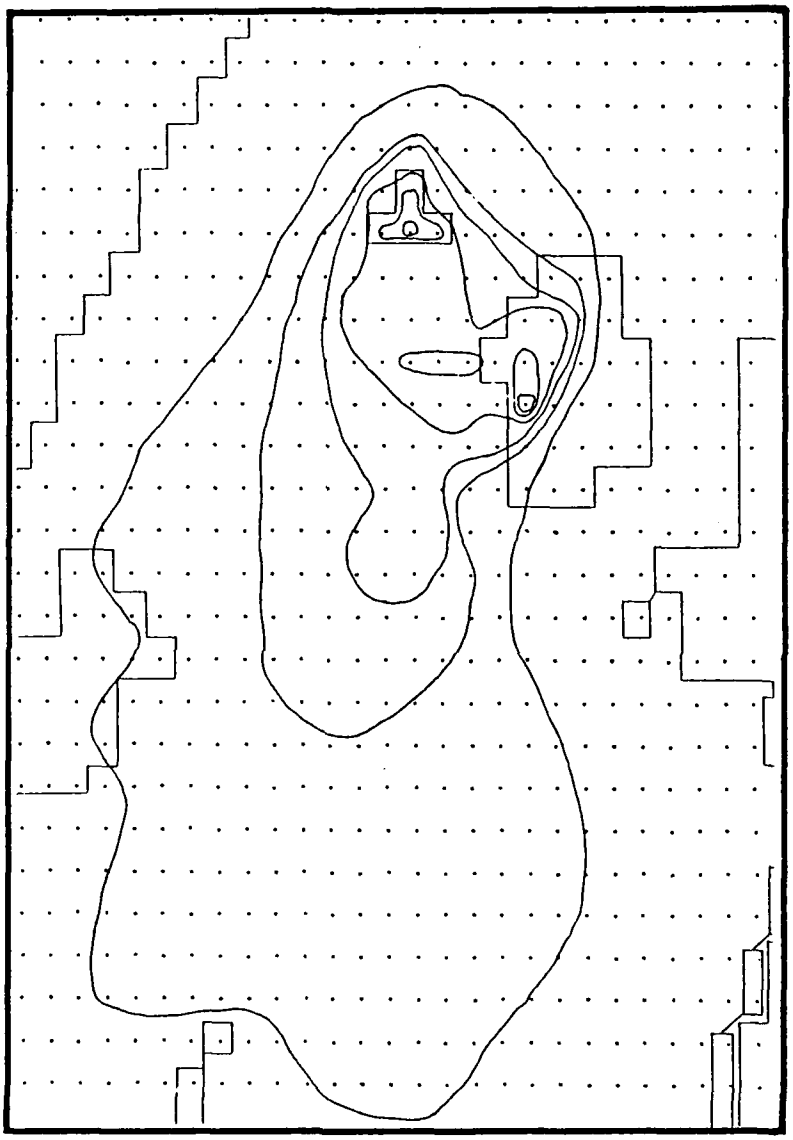

Figure 84. RW/Otis Plume Concentration Map for DISPL = 500 Ft.

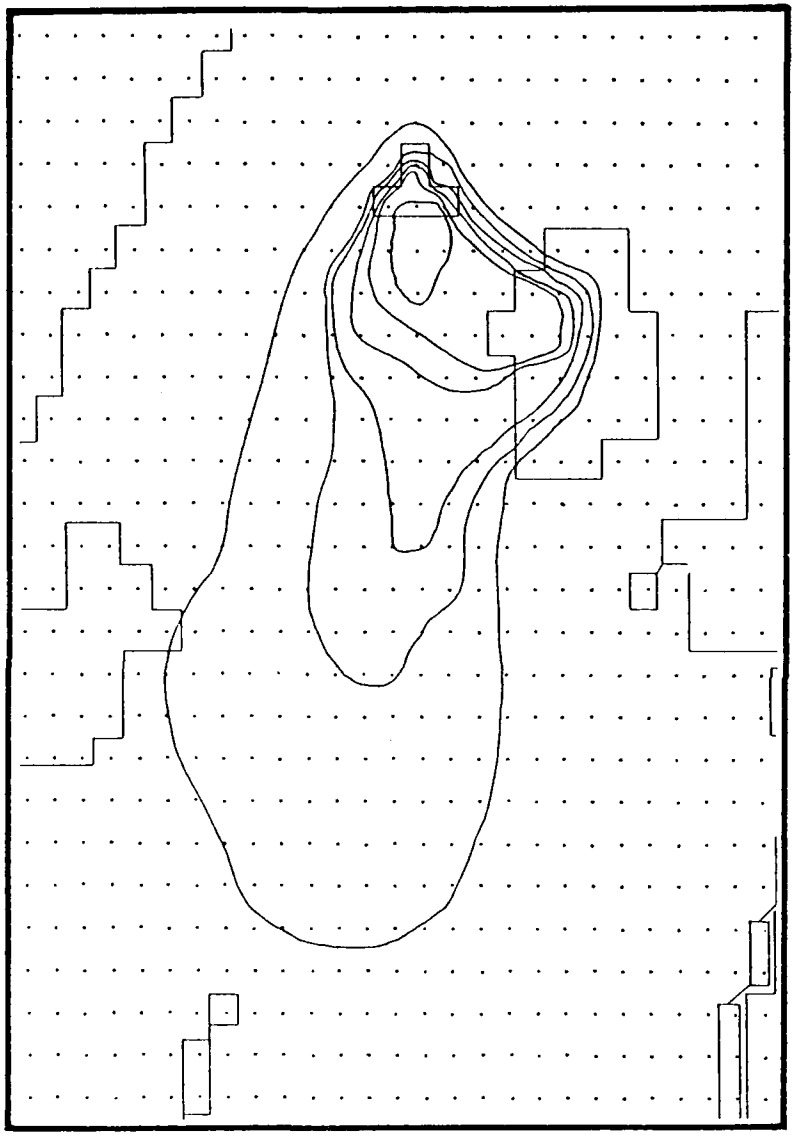

Figure 85. RW/Otis Plume Concentration Map for CONC = 600 ppb.

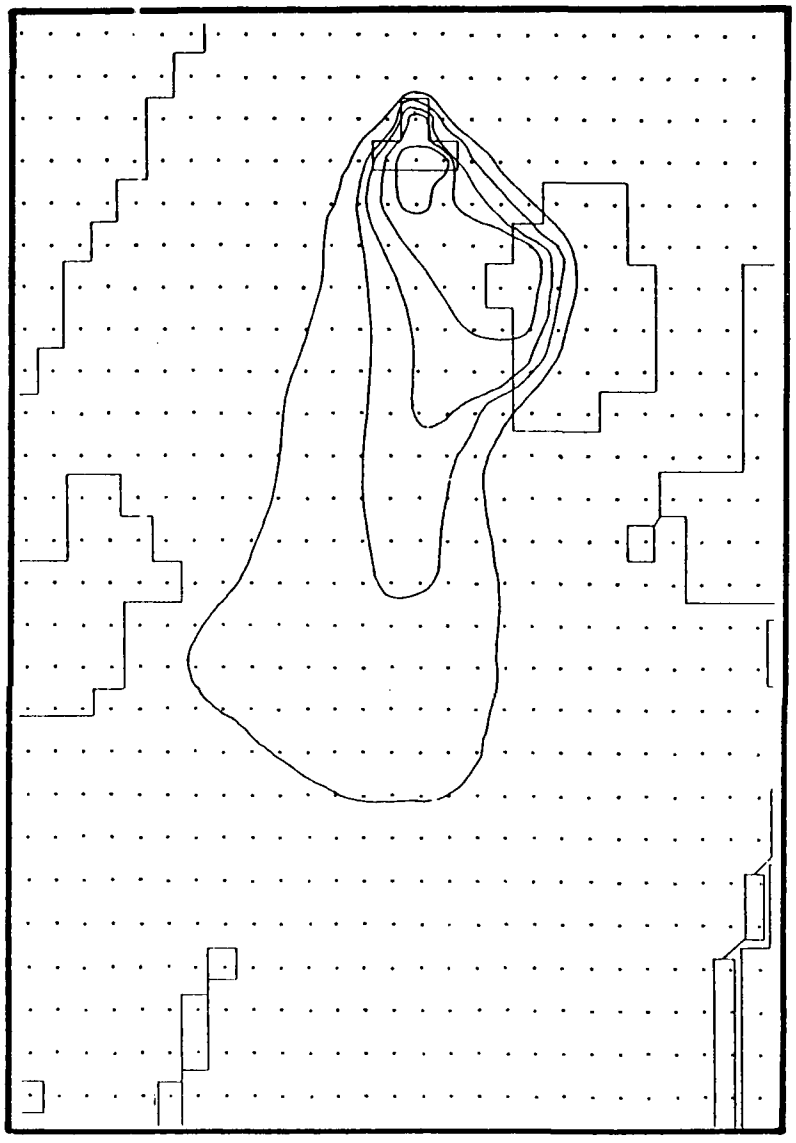

Figure 86. RW/Otis Plume Concentration Map for CONC = 400 ppb.

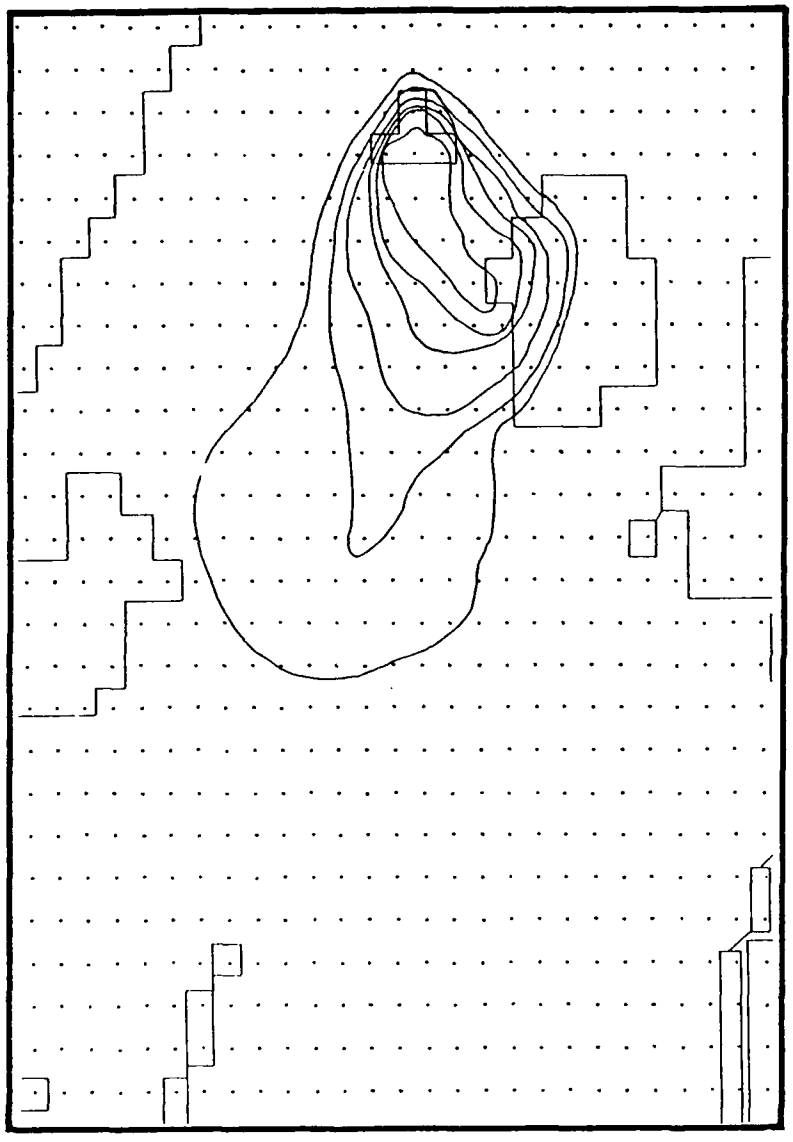

Figure 87. RW/Otis Plume Concentration Map for RD1 = 1.25.

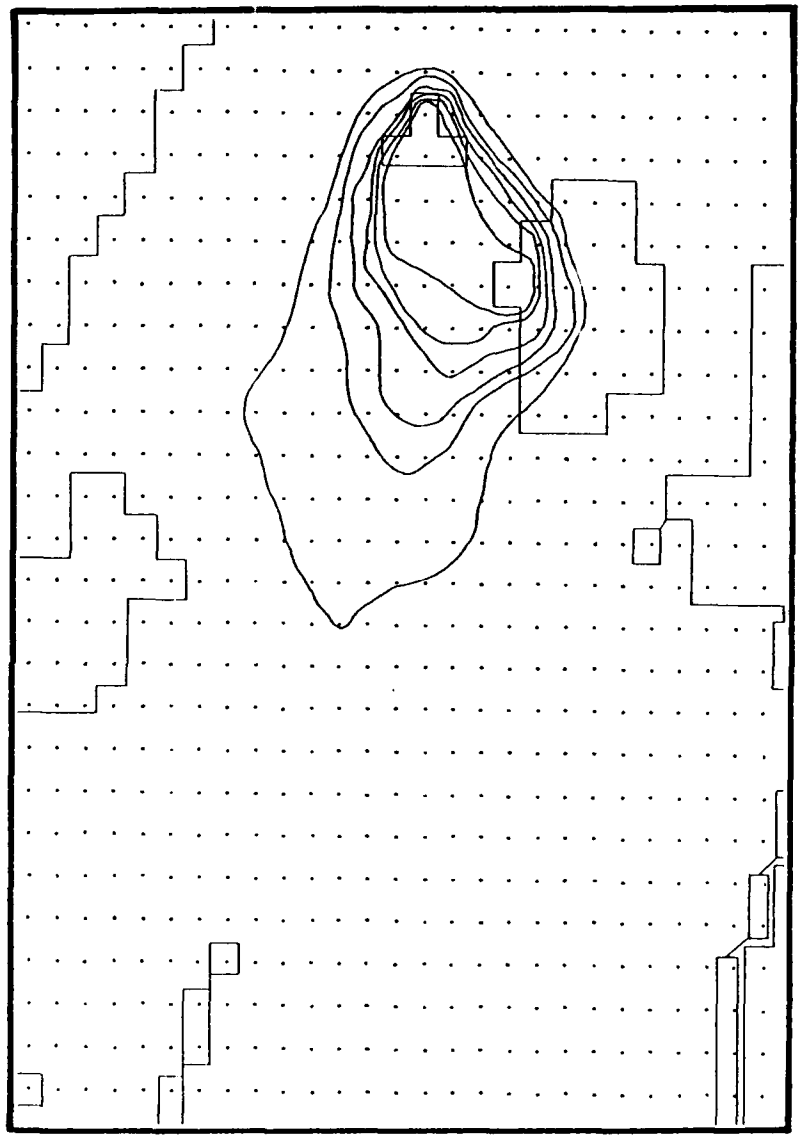

Figure 88. RW/Otis Plume Concentration Map for RD1 = 1.50.

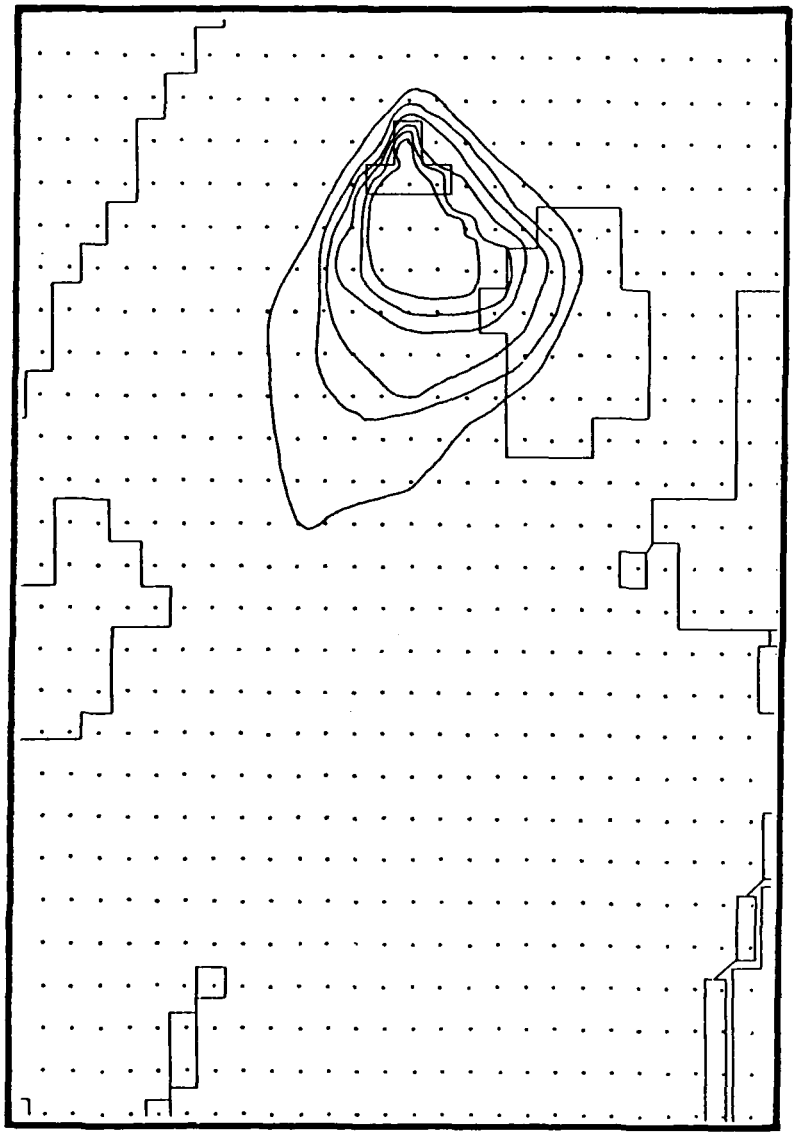

Figure 89. RW/Otis Plume Concentration Map for RD1 = 2.00.

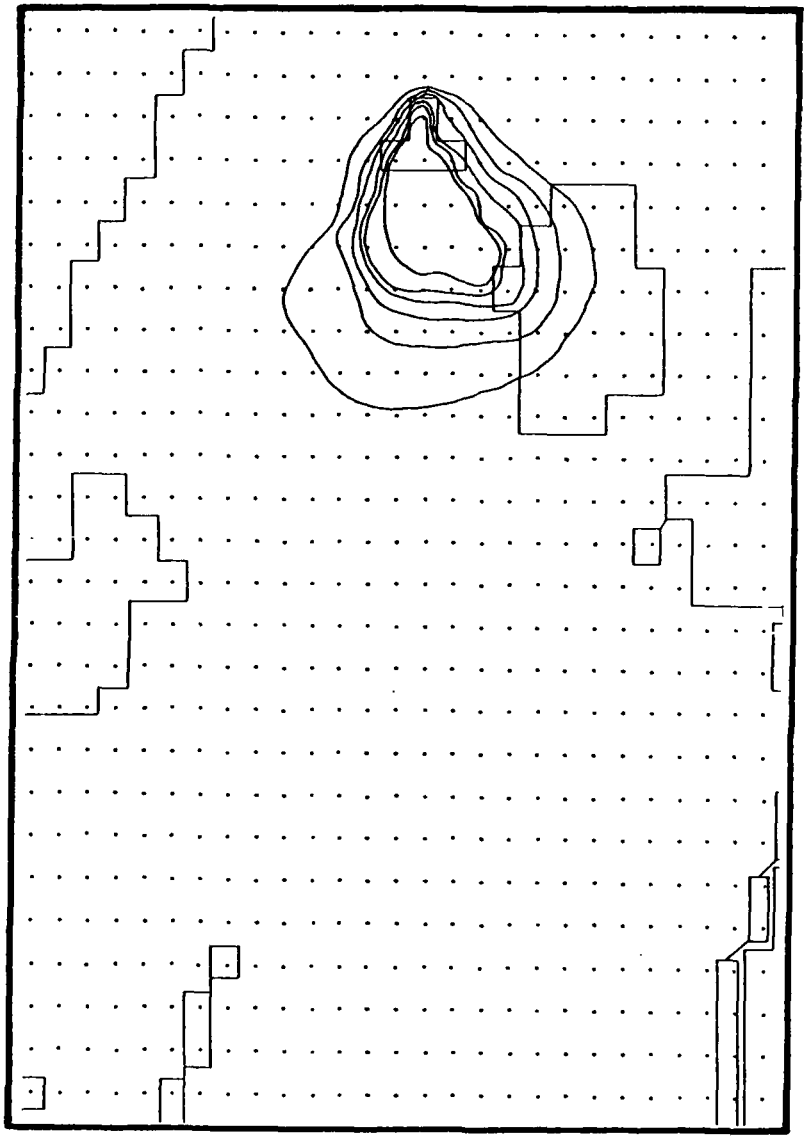

Figure 90. RW/Otis Plume Concentration Map for RD1 = 3.00.

In summary, the sensitivity study shows that the parameters can be divided into three categories. First, the following parameters either had no effect on the Otis results or were eliminated a priori from the sensitivity study: NSTEPS, NRT, X1, DX, Y1, DY, PL, T1(I,J), T2(I,J), H(I,J), NC, NR, DELX, DELY, NPUMP, CH(I,J), BOTT(I,J), RH(I,J), RD (I,J), NSP, S1(I,J). Second, the following parameters have little or no sensitivity effect, provided they are specified at an approximately correct value: R(I,J), DELTA, NPITS, DELP, ERROR, MAXP, DISPT, DXMAX, DYMAX, DISPT. Third, the following parameters had appreciable effects: PERM1(I,J), PERM2(I,J), Q(I,J), DISPL, CONSOR(I,J), RD1.

SECTION VIII

SIMULATION RESULTS USING SUTRA

A. INTRODUCTION

This section is divided into four discussions addressing the procedures followed during this analysis and implementation of the SUTRA model. First, for familiarization, the SUTRA-82 (Reference 7) test problems were run on the CYBER System and an input data template was prepared. Second, SUTRA-84 (Reference 8) was reviewed, and installed on the CYBER System. Then, its test problems were run and its input data template was prepared. Because of the complexity of SUTRA-84 and the limitations of the CYBER System, ways were examined to increase the core memory storage capability of the system for this version of the model. Third, input data files were prepared for the Otis sewage plume. Fourth, further analysis of the core memory requirements of SUTRA for the various sample problems and the Otis simulation was conducted.

B. INSTALLATION AND TESTING OF SUTRA-82

SUTRA-82, the October 1982 version of SUTRA (Reference 7), had been installed and run on the CYBER System before this project. The first step followed in this project was familiarization with the program through study of the User's Manual and running of the sample problems. The four sample problems considered in this analysis were:

- radial mass transfer from a well
- radial energy transfer from a well, actually adapted from the SUTRA-84 manual (Reference 8)
- salt water intrusion into a confined layer
- solute transport at Rocky Mountain Arsenal at Denver, Colorado.

All four test problems ran quickly and successfully. From the program source listing and the User's Manual, an input template was prepared. An annotated template is found in Appendix G, which lists the name, purpose and format of each input item; units of pertinent quantities; special cases; and other pertinent information.

C. INSTALLATION AND IMPLEMENTATION OF SUTRA-84

1. Installation and Testing

The installation and testing of SUTRA-84, the December 1984 version of SUTRA (Reference 8), required more effort than expended for SUTRA-82. Initially, the program was available only on tape. As before, the first step of familiarization was to study the User's Manual. Then, the source code was installed on the CYBER System. This version of the SUTRA source code required 26 separate files on the tape. For the CYBER System, these files were concatenated into one long source code file. Because SUTRA was originally written for use on a PRIME computer, certain system calls were changed to their CYBER system equivalents.

At this point, the program was ready to be tested. As before, the sample problems (previously listed) were used as test cases. Their necessary input data files were located on the file tape and the runs were made. These problems were essentially identical to those of the 1982 version except the input formats differed slightly, reflecting some changes in I/O coding. Three of the four problems ran successfully. However, the Rocky Mountain Arsenal problem ran unsuccessfully because the system's core memory availability was insufficient.

An annotated input data file template for SUTRA-84 is given in Appendix H.

2. Implementation

As with the Rocky Mountain Arsenal problem, the Otis sewage plume simulation requires enhanced core storage above that normally available to a specific user of the CYBER System. One possible option to overcome this deficiency is to edit SUTRA-84 to run in a single precision mode. Single precision is a reasonable option because the CYBER is a 64-bit mainframe computer. (For example, on a 16-bit PC system, double precision would be required.) A single precision version of SUTRA-84 has been prepared and successfully ran a sample problem.

A second option for solving the core storage problem of SUTRA-84 is the conversion of the two largest arrays in the core common storage (i.e., LGEM and LGEV) to tabular storage on a disk. Again, this option has been implemented and this version of the program was run successfully for a sample problem.

Tabular storage on disks has a major limitation, namely: disk access is much slower than core memory access. Thus, the run time for large problems will be greatly increased. Because of the CYBER System limitations, such runs would generally have to be made overnight, further lengthening turn around time for the large problems. Consequently, these problems could only be practically run on the CYBER with computational meshes moderately larger than those which core memory could handle alone.

Simulations of significantly larger meshes could not be completed in one night, and would have to be continued on successive nights. Fortunately, the SUTRA-84 program has a built-in "hot start" option to facilitate multinight runs. The administrator of the CYBER System would take an accommodating attitude toward such runs.

However, this option is useful when only a few multi-night runs are needed. Such runs could confirm that fine meshes are not required, or they could improve the resolution of selected plume maps generated by coarser mesh runs. It would not be feasible if most of the modeling runs for an aquifer required several nights. Since many simulation runs are usually required to model an aquifer, large, fine-mesh simulations will require a computer system larger than the CYBER at the AFESC.

D. INPUT AND OUTPUT DATA FILES

1. Input Data File for the Otis Simulation

As previously discussed, it was expected that the CYBER's core storage limitations would be exceeded if SUTRA was run for Otis using the 34 x 38 element array used for both the USGS-2D and Random Walk models. Thus, a coarser mesh was constructed over the Otis domain of computation. This may be a feasible approach for reasons other than just the size of the core memory. In some test problems, SUTRA has given more accurate results for the same meshes as used for finite-difference methods, although more CPU time is usually required. Thus, coarser meshes than used in the USGS-2D and RW models may result in SUTRA calculations which do not sacrifice modeling accuracy and CPU time requirements.

A 20 x 24 element mesh, shown in Figure 91, was prepared for the SUTRA-82 simulation of the Otis sewage plume. This grid features nonuniform elements having the following shapes:

- About two-thirds of the elements are rectangles.
- About one-third of the elements are trapezoids.
- A few of the elements are irregular quadrilaterals.

Further, the grid has 20 elements in each East-West row. These elements are equally spaced except in the vicinity of Ashumet Pond. The spacing in the North-South rows is either 1500 or 3000 feet. The input parametric values for the SUTRA-82 simulation of the Otis sewage plume are given in Appendix I.

Even with the 20 x 24 element mesh given in Figure 91, it was found that the core storage limitations of the CYBER System were exceeded.

2. General SUTRA Input and Output Files

Two input data files are required to run SUTRA. The main file is "UNIT-5", which contains the simulation control parameters, the mesh specifications, and the boundary conditions. The initial conditions are found in "UNIT-55." The requirements for these files are shown for the 1984 version in the 1984 User's Manual (Reference 8) in the form of an extended table. There is no comparable table in the 1982 User's Manual (Reference 7). Eight-page annotated coding templates have been prepared for both SUTRA versions and can be found in Appendices G and H of this report. Because the CYBER System was too small to model the Otis plume with SUTRA, these templates do not have as many detailed hints as found in the templates for the USGS-2D and Random Walk models.

E. SUTRA CORE MEMORY REQUIREMENTS

In this subsection, a more detailed analysis of CYBER core memory requirements for the sample problems and for the Otis simulation using SUTRA-82 and SUTRA-84 is given. Other core memory analyses are also given.

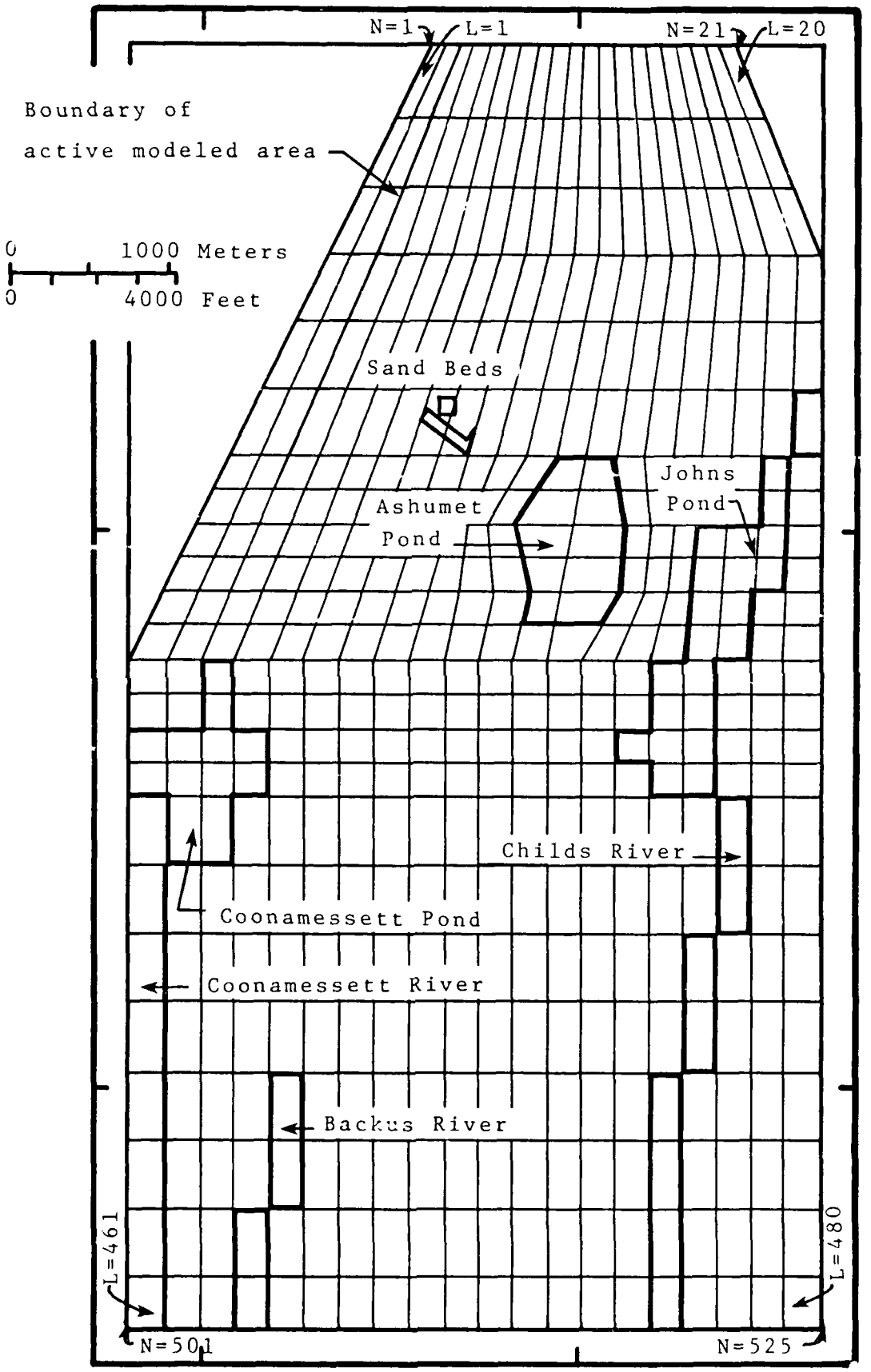

Figure 91. SUTRA-82 Grid Chosen for the Otis ANGB Sewage Plume.

1. Sample Problem Requirements

The core storage capability of the CYBER System is given as 375.1 kilobytes (KB) octal basis, which is equivalent to 129.6 KB decimal. In an attempt to meet this system requirement, the three solute transport sample problems (see Section VIII-B) were rerun on both the SUTRA-82 and SUTRA-84 programs with optimized COMMON (dimension) statements. When the storage for program overhead is added to the array common storage, the total storage requirement is exceeded in at least one configuration. Summary data from these reruns are shown in Table 12.

2. Otis Plume Requirements

Table 13 summarizes the core memory requirements for simulating the Otis sewage plume. The 20 x 24 element mesh requires about 170 KB (decimal) of core memory at double precision and the 34 x 38 mesh requires, correspondingly, about 570 KB. According to Dr. Voss an even finer mesh would probably be required to properly simulate the Otis plume using SUTRA, say something on the order of 50 x 80 elements. The core memory requirements for such a mesh would be on the order of 1 MB (decimal) for single precision accuracy. Thus, the use of an alternate computer system is required. For example, a VAX minicomputer, via telephone modem hookup, with at least 10 MB core memory would be feasible for this type of simulation.

3. SUTRA Mesh Discretization Limitations

Some calculations were performed to determine SUTRA mesh discretization limitations on the CYBER System. For 1-D meshes, an algebraic hand-solution using a linear equation indicated that the mesh could be up to 518 elements long for SUTRA-82 and 418 for SUTRA-84. For a 2-D rectangular mesh, the corresponding algebraic equation is nonlinear. Thus, short computer programs for SUTRA-82 and SUTRA-84 were prepared in GW Basic 3.2. These mesh discretization calculations and program code listings are given in Appendix I. These results and programs can be used by inexperienced users to determine mesh discretization limitations for the two SUTRA versions, as applied to various pertinent groundwater/solute problems.

TABLE 12. STATISTICS FROM SUTRA SAMPLE PROBLEM RUNS.

Version	82	84	82	84	82	84
Single/Double Precision	SP	DP	SP	DP	SP	DP
Elem/Row	1[a]	1[a]	10	10	16	16
Elem/Column	65	65	20	20	20	20
No. of Elements	65	65	200	200	320	320
No. of Nodes	132	132	231	231	357	357
Bandwidth	7	7	25	25	37	37
No. of Sources	2	2	11	11	4	4
No. of BCs	4	4	11	11	28	28
No. of Time Steps	450	450	100	100	30	30
CPU Time (sec)	981	327	1143	1344	438	b
LGEM[c] (KB_{10})	2.1	4.1	12.3	24.6	26.6	53.2
LGEV[d] (KB_{10})	5.1	12.3	9.2	22.5	17.4	34.8
LGEMV[e] (KB_{10})	1.0	1.0	1.0	2.0	3.1	6.1
Program Overhead (KB_{10})	24.6	30.7	24.6	30.7	24.6	30.7
Total Storage (KB_{10})	32.6	48.1	47.1	79.8	71.7	124.8[g]
KB_8[f]	100	136	134	234	214.0	363.6

a 1-dimensional.

b Aborted.

c Storage requirement for real matrices in common, expressed in KB (decimal).

d Storage requirment for real vectors in common, expressed in KB (decimal).

e Storage requirement for integers in common, expressed in KB (decimal).

f Total program storage requirement in KB (octal).

g Because this run aborted and this "total" appears to be less than 129.6 KB (decimal), some requirement(s) were mistakenly not included in this "total".

TABLE 13. CORE MEMORY REQUIREMENTS FOR VARIOUS OTIS/SUTRA GRIDS.

Version	82	84	82	84	82	84
Single/Double Precision	SP	DP	SP	DP	SP	DP
Elem/Row	20	20	34	34	50	50
Elem/Column	24	24	38	38	80	80
No. of Elements	480	480	1292	1292	4000	4000
No. of Nodes	525	525	1365	1365	4131	4131
Bandwidth	45	45	73	73	105	105
No. of Sources	26	26	27	27	50	50
No. of Const P/U BCs	50	50	87	87	200	200
LGEM (KB_{10})[a]	48	95	201	403	870	1741
LGEV[b]	20	38	49	131	150	398
LGEMV[c]	5	10	12	25	37	74
Program Overhead	18.5	31	19	31	19	31
Total Core (KB_{10})	91.5	174	281	590	1075	2245
K (KB_8)[d]	263	524	1045	2200	4060	10440

a Storage requirement for real matrices in common, expressed in KB (decimal).

b Storage requirment for real vectors in common, expressed in KB (decimal).

c Storage requirement for integers in common, expressed in KB (decimal).

d Total program storage requirement in KB (octal).

SECTION IX

MODEL COMPARISON

The objective of this study was to test and evaluate the three groundwater solute transport models available for use on the AFESC computer. These tests and evaluations were conducted to identify problems involved with modeling real field data on AFESC hardware, to compare the simulation accuracy and the relative benefits and limitations of each of the three models, and to test the sensitivity of various input parameters.

The following are topics considered in this section: limitations uncovered during the model simulations, comparison of model sophistication, input data requirements, readability of model results, model accuracy, and CPU time and storage requirements.

A. LIMITATIONS IDENTIFIED DURING MODEL RUNS

Running the three models on field data uncovered several limitations of the available data sets and a crucial limitation of the CYBER Computer System for running such models against such data. These limitations are outlined in the following paragraphs.

1. Three-Dimensional Effects

All of the models tested are two-dimensional (areal simulation) models which assume constant and/or vertically-integrated parameters and variables over the depth of a groundwater/solute system. However, field measurements of the Otis sewage plume detected appreciable vertical stratification in some areas, which may have led to the degradation of model accuracy in the current simulations.

2. Solute Material Balance

The formulations of the groundwater solute models allow solute to pass into a body of water (e.g., Ashumet Pond in Figure 31), but do not allow the solute to properly mix in that body and do not allow the solute to reenter the aquifer in regions where the hydraulic gradient permits. Hence, strategically placed water bodies (e.g., Ashumet Pond in Figures 36 and 37) become exaggerated solute sinks. This problem can be corrected through the addition of subroutines to account for proper mixing of the solute dissolved in ponds and lakes and its reentry into the aquifer by the specification of time-dependent solute source cells.

3. Coarseness of the Discretization

The CYBER core memory was too small to allow proper testing of the effects of mesh size on pollutant plume dispersion. Thus, it was impossible to properly assess the effects of the numerical dispersion produced by the USGS-2D model versus that produced by the Random Walk model (numerical dispersion of the RW model should be much less than that of the USGS model). In addition, the coarseness of the mesh did not allow the Otis plume to be properly modeled by either the SUTRA-82 or SUTRA-84 programs.

The "Calibration" phases of the USGS-2D and Random Walk models revealed that best plume fits were given when the longitudinal dispersivity for the RW model was larger than that used by the USGS-2D model, larger by a factor of 2 to 4. This difference may have been due to the "numerical dispersion" differences between the two models; but, as stated, the CYBER's core memory limitation prevented a definitive test of this proposition.

4. Masking of Errors

Because of the inadequacy of certain site data and the limitations of the CYBER system, errors in certain parameters and formulations of physical phenomena may have gone undetected and/or unsubstantiated because of "error-masking." Such masking of errors in parameters and phenomena which simultaneously affect output results may produce relatively accurate plume simulation maps from distorted input data. Two possible examples of such masking in the Otis simulation are as follows:

- The lack of accounting for vertical stratification versus the inaccurate specification of Ashumet Pond leakage.
- Improperly accounting for the interaction between hydraulic conductivity effects and rainfall recharge effects.

5. Variable Solute Source

For modeling, the Otis solute source was taken as constant over the 40-year simulation period. However, Figure 33 shows that this was not the case. Source rates were probably much higher in the 1940s and the 1960s than in recent years. The assumption used in the simulation of the Otis plume may have possibly given a shorter plume than reality and may have altered the width of the plume as well.

6. Unavailable Data

Certain unpublished data on aquifer thicknesses and river levels possibly used by LeBlanc in his analyses, were not available for this study. The availability of such data may have improved the overall results of the model/field testing program. At least, confidence in the results from the simulations would have been enhanced.

B. MODEL SOPHISTICATION

In considering "model sophistication," as well as the other characteristics, both the size and complexity of the Otis simulation and the limitations of the CYBER System are, and must be, taken into account.

1. USGS-2D and Random Walk Models

Both the USGS-2D and Random Walk models, as previously stated, use fixed-coordinate, alternating-direction implicit procedures for obtaining groundwater head solutions. Both programs use moving particle routines for solute advection, sources, and sinks. The programs differ in simulating dispersion, adsorption and chemical reactions or species decay. In the USGS-2D model, many calculations involving the moving particles are referred

to fixed coordinates; while in the RW model, the analogous calculations or phenomena are made and analyzed in the moving frame of reference.

a. Solute Dispersion Effects

Solute dispersion effects in the USGS-2D program are determined using nodal concentrations and specified dispersion coefficients, while the RW program simulates dispersion by a random walk process. Thus, the RW program runs with less core storage than the USGS-2D program and permits the accumulation of plume maps from repeated runs. However, the conversion back to fixed coordinates in the USGS-2D model gives this model more flexibility in adsorption and reaction formulations than the RW model.

b. Adsorption Rate Calculations

Adsorption rate calculations in a stationary frame of reference generally involve adsorption isotherms, which relate fractional saturation of the solid phase with the aqueous phase solute concentrations. The 1982 version of USGS-2D (Reference 4) includes optional calculations for three different adsorption isotherms.

Random Walk algorithms, with their moving frame of reference, cannot generally use the isotherm formulations. Instead, the RW model uses the retardation-factor concept. In this concept, adsorption is considered to be a storage phenomenon, where solute accumulates in both the aqueous and adsorbed phases. The extra storage capacity of the adsorbed phase "retards" the spread of the contaminant plume. The retardation factor, which quantifies this phenomenon, acts as a linear adsorption isotherm. Fortunately, the low solute concentrations found in most groundwater situations can be analyzed in terms of linear isotherm adsorption mechanisms.

c. Chemical Reactions/Species Decay

The 1982 version of the USGS-2D (Reference 4) model allows the solute content of each solute "particle" to change independently, thus allowing USGS-2D to track rather complex homogeneous and heterogeneous chemical reactions, and species decay. On the other hand, the RW program cannot handle most reactions/species decay in a rigorous manner. However, for linear (or first-order) reactions and decay (nuclear or biological), the RW program can easily accommodate the situation. For example, for each time increment and tracer particle, the particle mass PM can be decreased by a constant factor to account for the chemical reaction or species decay, since linear rates are independent of solute concentration or particle mass.

For nonlinear kinetics, reaction/decay rates are particle- or mass-dependent. Thus, the bookkeeping required to adjust retardation factors for each particle and each time step in order to empirically match field concentration values would be extremely complex and CPU time-consuming, and may not even be well-supported theoretically. Consequently, the USGS-2D model is generally superior to the RW model for chemical reaction/species decay formulations.

d. The Otis Experience

For the Otis simulations, neither model showed a clear overall advantage over the other with respect to model sophistication. For both models the discretizations were the same. The RW model can use more particles within the constraints of the CYBER System than the USGS-2D model, and thus can produce slightly smoother plume concentration maps. Since this study did not consider the phenomena of adsorption and chemical reactions, the disadvantages of the RW model in this regard were not emphasized.

2. SUTRA Model

The SUTRA model has options that enhance the simulation of groundwater solute transport. Some of these features are as follows (References 7, 8):

- energy transport simulations,
- unsaturated flow simulations,
- hot restart capability,
- pressure boundary value conductance,
- density driven flows,
- optional adsorption parameters,
- reaction kinetics parameters,
- gravitational effects on non-horizontal flows,
- time variation of hydraulic head boundary conditions,
- nonrectangular discretization, and
- specification of anisotropic permeability and dispersivity.

Whenever flexible element shapes are required, the finite-element formulation used in SUTRA is very attractive. Even though useful for Otis (Figure 91), this flexibility was not really required in this study. However, the achievement of comparable accuracy and possible comparable CPU time with fewer grid elements than required by USGS-2D and RW should be a definite plus for the SUTRA formulation in some specific applications. A feature that could be added to SUTRA-82/SUTRA-84 for use in sites analogous to the Otis site is a module that would allow the specification of leaky artesian boundary conditions.

C. INPUT DATA REQUIREMENTS

The USGS-2D and RW programs have very similar input data requirements, while SUTRA requires considerably more data. The USGS-2D model uses a data map for each of several parameters, while the RW model uses a "Node Card Deck," that is a single table for all data specified by node. SUTRA stores its input data in tables and reads data from several different tables. In

general, data maps (USGS-2D) are more convenient for smaller aquifers (i.e., smaller grid networks), and the user can comprehend these maps easier than tabulated data. The data tables generally have an advantage if most of the properties are uniform across the aquifer, because lines of data are entered only for nodes with nondefault parameter values.

For the Otis simulation, the USGS-2D input data files were considerably shorter than the RW files because a complete line of RW data had to be specified for each cell where a non-default value is required for even one input parameter. Most cells (i.e., 820 out of 1292) in RW needed to be specified because there was no aquifer-wide default value for cell bottom elevation. The parameter sensitivities of the USGS-2D and RW programs were similar. The USGS-2D model clearly showed sensitivity to cell thickness, hydraulic conductivity, rainfall recharge rate, sewage concentration, sewage flow rate, and porosity. The RW model clearly showed sensitivity to the preceding parameters plus longitudinal dispersivity, "capture radius," and retardation factor.

D. READABILITY OF MODEL RESULTS

In general, none of the three models are currently implemented on the CYBER System to give high-quality pollutant plume maps. Their current status and readability potential are given in the following paragraphs.

1. USGS-2D Program

The USGS-2D program calculates and stores the results for hydraulic heads and concentrations in map arrays, using cells of rectangular shape and uniform size. The line printer plots of head and concentration are handled by the source code. The simplest case is where rows of head and concentration data can each be printed on one line-printer output row. Otherwise, the maps can be printed blockwise, cut and pasted together by hand, and reproduced on a reducing copying machine. The continuous, fanfold line-printer paper can handle an arbitrary number of rows in the printout.

If computerized contouring and plotting of the head and concentration maps are desired, one version of USGS-2D available in the HQ AFESC/RDV program library interfaces between the CYBER System and a CALCOMP plotter.

2. Random Walk Program

Head and concentration maps for the RW program are printed from data storage arrays. If the cell size is specified as uniform (as in the Otis simulation), preparation of line-printer plots is analogous to USGS-2D plots. If variable cell dimensions are specified, line-printer maps can still be prepared. Since all the cells in any given column must have the same width, only one format statement is required for the rows. If cells in different rows have different lengths, different numbers of blank lines must be placed between the rows of printout. The overall scale must be chosen so that the physically narrowest cells still appear legibly in the printout. If the total number of characters (including blanks) per row exceeds 137, the map will be printed in blocks, as in USGS-2D.

No interface program has been written, to date, linking RW simulation maps to the CALCOMP plotter. While plotting might be a little more complicated than with USGS-2D due to the variable cell size, the added difficulties will not be major.

3. The SUTRA Program

Storage of head and plume data in the SUTRA program is somewhat different from the other two models. SUTRA's mesh can be of arbitrary geometry, as opposed to the rectangular grids of the USGS-2D and RW models. Thus, output data maps must be stored in the computer in table form, instead of array form. Consequently, SUTRA includes a subroutine PLOT to calculate and print line-printer plots from the tabular data.

The maps prepared by PLOT will often have a format acceptable to the user. Thus, in the input data file, the user can choose one of the printout format options offered by the source code. If necessary, the user can edit the source code of subroutine PLOT to formulate additional printout formats.

E. MODEL ACCURACY

No major differences were apparent between the simulation results of the USGS-2D and RW programs. The SUTRA program was not adequately tested on the Otis simulation, so no definitive statements regarding model/model or model/field comparison can be made for this system. Thus, the remaining comments in this subsection only refer to the USGS-2D and RW models as applied to the Otis ANGB data.

The USGS-2D and RW programs, in general, appeared to give useful and reasonably accurate overall simulations for head and concentration maps based on the input and output information published by LeBlanc (References 17, 18). Exceptions to these statements are as follows:

- The head simulation was moderately in error over the northernmost portion of the computational domain for Otis. Fortunately, the effects of this error were localized; but the presence of the error still leaves unresolved questions concerning the simulations.

- To produce comparable maps for Otis by the USGS-2D and RW models, the longitudinal dispersivity parameter was increased for the RW model compared to that used by the USGS-2D model (a value comparable to that used by LeBlanc). A possible explanation of the necessity of doing this was given in Section IX-A-2-c.

The two greatest weaknesses with these models in simulating the Otis sewage plume are the inabilities of the models to account for vertical stratification and the changing source concentrations at Ashumet Pond. These weaknesses degrade the accuracy and resolution of the final head and solute concentration results obtained from the models. In general, vertical resolution can only be enhanced by going to three-dimensional simulations, with their increased computer storage and CPU time requirements. The Ashumet Pond solute sink/source problem could be accounted for with less effort; however, significant code modifications of the current models would still be anticipated.

Generally speaking, the key to an accurate simulation is the ability of a given model to accurately represent the hydrological system under study within the resource limitations of the computer system. Questions which require answers in such an assessment are as follows:

- Is adequate discretization possible given the physical system to be modeled and the available computer system? In the case of the applicability of SUTRA for Otis using the CYBER System, the answer is no.

- Does the model contain input data features and internal structure adequate to represent the pertinent aquifers, rivers, ponds, and other features, and the corresponding boundary conditions? In the study, the models gave adequate areal resolution of long-term pollutant plumes, but only marginal vertical resolution of the contaminated area.

- Are the models' solution algorithms adequate for the "task at hand?" Algorithmically speaking, finite-element models are often superior to finite-difference/particle models for groundwater/solute simulations. However, in this study, for the generation of areal head and solute concentration maps, the USGS-2D and RW models proved superior to the SUTRA models (for reasons that have already been stated).

F. CPU TIME AND STORAGE REQUIREMENTS

For the base case runs of the USGS-2D and RW models on the Otis sewage plume, the following CPU times and storages were required:

Parameter	USGS-2D	Random Walk
Compilation Time (Seconds)	17.5	8
Maximum Execution Storage (KB, octal)	275	205
CPU Execution Time (Seconds)	405	750

As previously stated, SUTRA requires considerably more data storage capacity and longer run times for a given discretization than do the other two models. However, the accuracy and efficiency of the finite-element formulation may allow coarser discretizations, and resultant decreases in CPU times and decreases in storage requirements, thus, reducing some of the disadvantages that SUTRA appears to possess over the other models in the current studies.

SECTION X

GENERAL CONCLUSIONS AND RECOMMENDATIONS

Groundwater/solute modeling is a useful tool for evaluating the representativeness and comprehensiveness of sets of field data, for predicting the long-term migration paths of contaminated groundwater plumes, and for planning and evaluating various remedial action options at contaminated sites. Modeling, along with sufficient field data, can play a very important role in locating in time and space, and thus in optimizing over time and space, the locations of detailed well and bore-hole fields for both the gathering of field data for more comprehensive and accurate groundwater/solute assessments, and for the control of contaminant plumes by employing discharging and recharging well fields.

Application of modeling methods may be both necessary and cost-effective in the USAF's IRP activities. Some of the areas of application include:

- Assessing the need for any remedial action at a given contaminated site, answering the question, "Will the contaminated plume eventually leave the AF site in question?"

- Determining when a given remedial action should be implemented at a site and determining the extent of this action and the physical location of wells, barriers, etc.

- Estimating the optimal pumping and recharge rates and durations of the activities for plume control by well fields.

For the models (i.e., USGS-2D, Random Walk, and SUTRA) evaluated in the current study, it is believed that the USGS-2D and RW models are useful in carrying out the above AF IRP activities if the site's hydrogeology is reasonably consistent with the models' assumptions. SUTRA may be better suited for certain research studies than for IRP remedial planning. For comparable discretization, SUTRA requires more data input, more CPU run time, and more core memory, but still lacks some source code features which would be very attractive for some applications.

Site hydrogeology for which all three of the evaluated models will be most applicable includes the following features:

- Groundwater should flow primarily through a homogeneous system of pores. Heterogeneities offering long, preferential flow paths, such as buried river bed gravel deposits or long rock fractures, are often not amenable to these groundwater models.

- Either the transport properties of the aquifer should be relatively uniform overall, or the input data file for the program used should be capable of effectively representing moderately varying properties using equations, arrays, or tables. The properties most commonly required in the input files are permeability, porosity, dispersivity, and aquifer thickness.

- The aquifer should be nearly horizontal, or the program should account for the gravitational effects of a moderately sloping flow field.

- The aquifer should exhibit saturated flow, unless the modeler has the additional data and time required to analyze unsaturated flow (e.g., in the SUTRA model).

- The contaminant sources should be reasonably well-defined and must be effectively represented in the input data file.

- The groundwater flow should be two-dimensional. This is a common initial assumption. Sometimes, as in the Otis sewage plume, appreciable vertical stratification is found, but useful simulations can still be achieved.

- The required input data must be available. Groundwater models are only as good as the underlying assumptions made and the input data used. For 2-D modeling, head and concentration input data must be taken over a well-defined areal pattern.

It is recommended that if significant three-dimensionality exists in the site for which modeling will contribute positive results, then the investigator should use systems other than those evaluated in this study. Several three-dimensional systems exist, many of which have been supported and developed by U.S. EPA, U.S. DOE, and EPRI funding. Ongoing evaluations of groundwater/solute models are taking place at the International Ground Water Modeling Center of the Holcomb Research Institute, Butler University, Indianapolis, Indiana (Reference 20). By keeping abreast of these evaluations, investigators in the USAF IRP can decide if one of the current models is applicable to a given site, or if a more detailed, three-dimensional system is required.

To upgrade groundwater/solute capability, it is further recommended that access to a computer with more core memory per user be obtained (e.g., dedicated, single-user VAX systems; time-sharing with larger mainframe computers; or use of a dedicated IBM PC with a math coprocessor chip, extended core memory and a UNIX operating system). Finally it is not recommended that extensive funding be supplied to develop new and more comprehensive, three-dimensional models for IRP application. However, a reasonable expenditure of funds may be the modification of some current 3D-models for efficient use on large memory, desktop computers for evaluation of contractor-proposed cleanup options.

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APPENDIX A

TOPOGRAPHIC MAP OF THE NORTHERN HALF OF THE OTIS SEWAGE PLUME

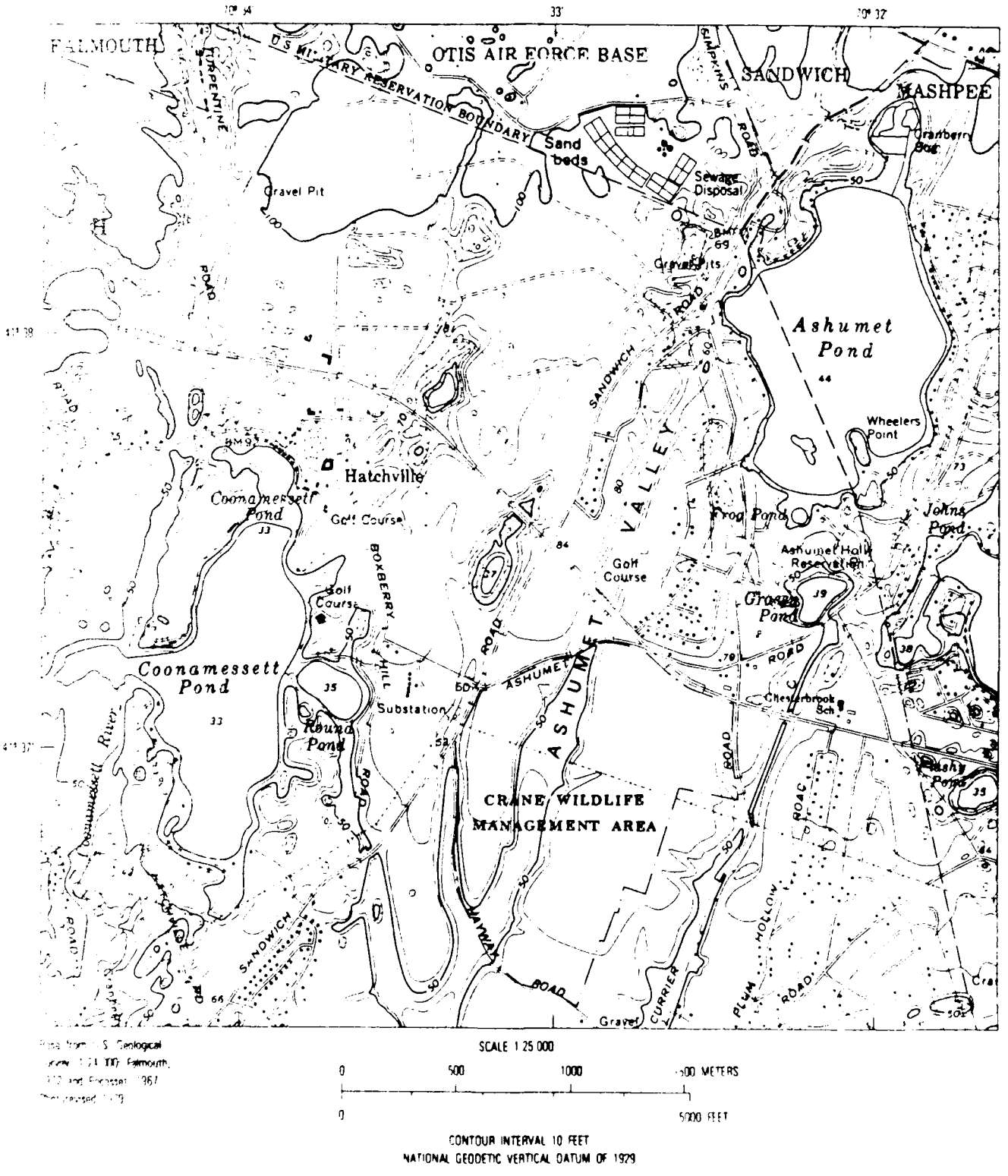


Figure A-1. Topographic Map of the Northern Half of the Otis Sewage Plume (Reference 1).

APPENDIX B

WATER TABLE MAP OF THE NORTHERN HALF OF THE OTIS SEWAGE PLUME

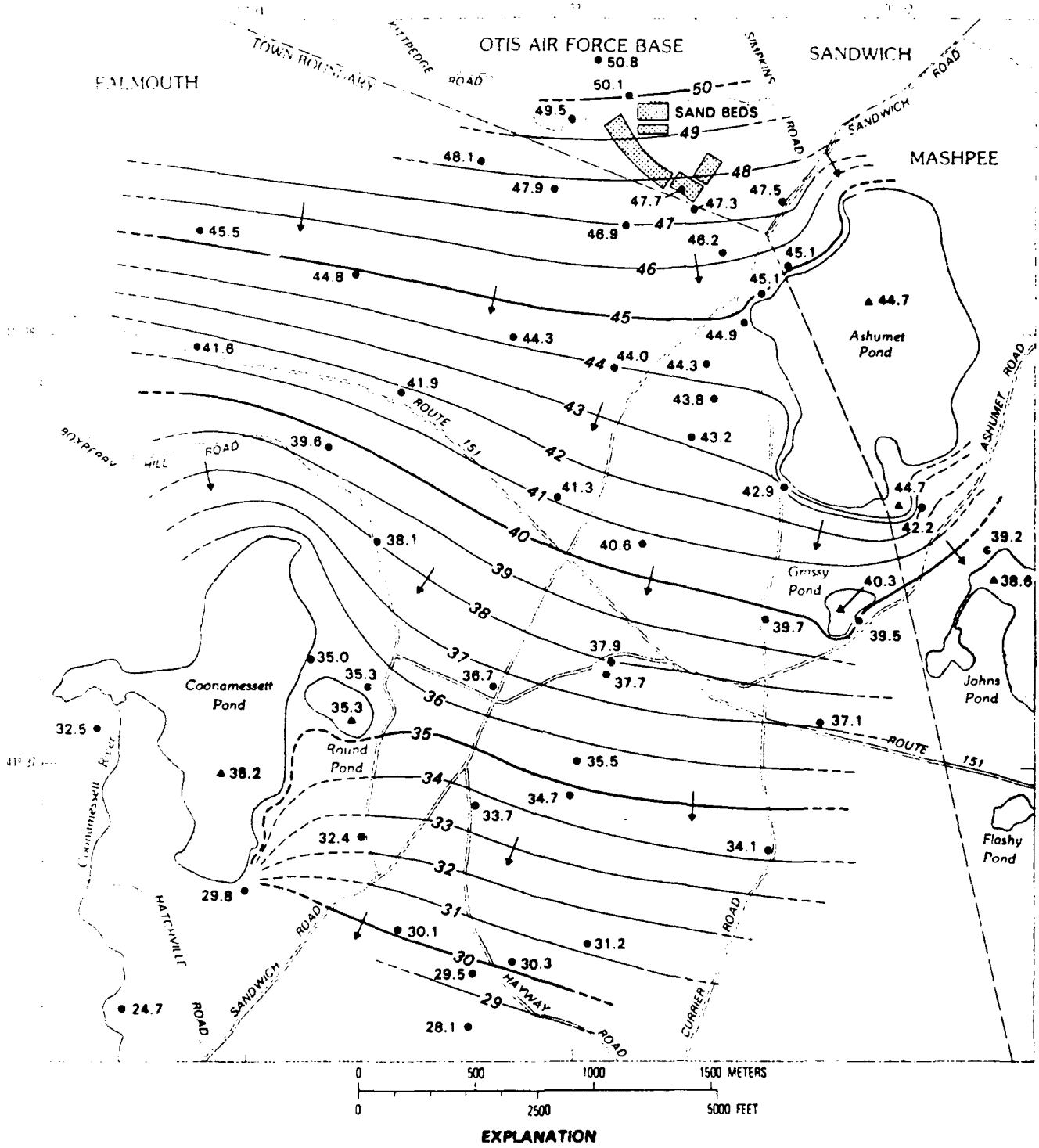


Figure B-1. Water Table Map of the Northern Half of the Otis Sewage Plume (Reference 1).

APPENDIX C

ANNOTATED INPUT DATA FILE TEMPLATE

FOR USGS-2D PROGRAM

APPENDIX C

NOTES ON SPECIFICATION OF INPUT PARAMETERS FOR USGS-2D RUNS

GENERAL REMARKS :

Note the abbreviations :

SS = steady-state groundwater flow (generally, solute transport will be unsteady-state)

USS = unsteady-state groundwater and solute flow

The default value is used by the program when a parameter is left blank in the input data file.

The finite difference grid is set up with the nodes centered in the blocks ("block-centered nodes"). Therefore, the words "block," "cell," and "node" can often be used interchangeably.

The words 'card' and 'line' (of data) will be used almost interchangeably.

- The program was originally written for punched card data input.
- It has since been revised to accept interactive terminal data input.
- All lines of data can be entered in an 80-column format, though many lines in the data sets would require continuation lines.
- The CYBER system can accept input data in formats of up to 136 columns

Data will be entered as "cards" and "data sets."

- a "card" (card image) is only one line long (<= 80 characters)
  - Values pertain to the entire equifer. (Data Set inputs may be specified on a block-by-block basis.)
- a "data set" may exceed one line in length, and often does.

Cards # 1 - 3 and Data Sets 3 - 9 are required. The other data are optional, and may be deleted.

An input template containing sample data and format requirements will be shown for each line and data set.
Explanatory text for each line is located below the corresponding template line.
Appendix D is the full input file for the case simulation of the Otis ANGB Sewage Treatment Plant Plume.

CARD # 1 TITLE :

Strongly recommended, in order to distinguish between runs, to avoid confusion and possible mislabeling of runs and printouts.

- however, the program will run properly with a blank title
- if a title longer than one line is required, the source code could easily be modified.

Title of run. Sufficient for positive ID of run.
10A8

- on the CYBER system, both its terminal and line printer, the maximum line length is 136 characters
- the current title format is (nA8), where n is the number of 8-character alphanumeric fields required.
- On the CYBER, the individual field lengths could be anywhere from A1 to A10.
- Default = a blank title line

CARD # 2 INTEGER PARAMETERS :

GENERAL
- This card contains 12 integer parameters
  - all are of format I4 (except I5 for NPMAX)
- These parameters will be specified once, on CARD # 2, for problems with steady-state heads
- When pumping rates will change over time, many of these parameters are re-specified for each "pumping period" on Data Set # 10, card B.

NTIM		NX		NPMAX		NITP		ITMAX		NPTPND		NPNTMV		NPNTD	
	NPMP		NY		NPNT		NUMOBS		NREC		NCODES		NPNTVL		
I4	I4	I4	I4	I5	I4	I4	I4	I4	I4	I4	I4	I4	I4	I4	

NPDELC

NPNCHV

I4 I4

- NOTES ON PARAMETERS :
  - **NTIM** : number of time steps per pumping period.
    - [SS] >= 1
    - [USS] >= 1
      (1 is simplest to use, but NTIM > 1 may speed convergence in unsteady-state flow cases.)
    - Default value = 1
    - Minimum value = 1
    - Maximum value = 100 (unless appropriate common statements in the source code are redimensioned higher).

- **NPMP** : number of pumping periods.
  - [SS] = 1
    (and omit "DATA SET # 10" input data file.)
  - [USS] >= 2
    (will require additional data sets in "DATA SET # 10".)
  - Default value : 1

- **NX** : Number of columns of blocks (nodes)
  - (For both [SS] and [USS] problems) :
  - Minimum = 3 (for 1-D problems)
    - setting this number too low (in 2-D problems) will hurt the accuracy of the simulation due to both NUMERICAL and MODELING THEORY considerations.
  - Maximum :
    - no theoretical limit
    - practical limit set by the computer system & time constraints (The practical limit on the CYBER is 40 - 50.
  - NX must not exceed the limits specified in the program in relevant DIMENSION statements
    - The program arrays were originally dimensioned at 20 x 20
    - If NX is substantially smaller than the common block dimensions, the user can readjust the relevant DIMENSION statements down for increased run time efficiency.
    - If NX > 20, redimension the source code, or the program will abend at execution time.
    - Default value : none

- **NY** : Number of rows of blocks (nodes).
  - See notes in NX.
  - NX OR NY should exceed 3.

- **NPMAX** : The maximum number of particles used in the simulation.
  - USGS originally set the dimension (length) of the particle arrays at 3200.
  - Users may prefer 5000 - 10000 particles in aquifer, for smoother, more accurate results.
  - The particle arrays in the source code can easily be redimensioned (in ALL appropriate subroutines) by the user
  - The actual number of particles in use will NOT change much during a simulation, even if there is a net injection of solute.
  - To maximize efficiency :
    - set NPMAX slightly but safely above the actual maximum number of particles used in the simulation
      (an excessive number of particles would reduce the efficiency of the program)
    - set the particle array DIMENSION statements slightly but safely above those required to hold NPMAX particles.
  - Do NOT **Underdimension** the particle arrays, or the program will abend at execution time.
  - With too few particles, the accuracy, precision, and readability of the results will suffer.
  - No **Default** value : the computer will read 0 and abor run.

- **NPNT** : Time Step Interval for printing Hydraulic and Chemical Output Data
  - Options :
    - May want to use 1 (frequent printouts for debugging or for calibrating steady-state cases.
    - May want to use higher values later on
    - Default value : none (program will abend)

- **NITP** : number of iteration parameters
  - Specifies the number of parameters used in the alternating direction implicit procedure, ADIP, the head solution subroutine
  - User's manual recommends a value of 4 to 7
  - Default value = none (program would read in 0 and abend)
  - Minimum value = 2 (or the program would abend)
  - Maximum value = 20 (or the appropriate arrays must be redimensioned)

- **NUMOBS** : number of observation wells
  - None are required
  - Maximum = 5
  - Default = 0 = minimum
  - If 0 is specified (or used by default) the program will **NOT** attempt to read a Data Set # 1. In this case, skip Data Set #1 in the input data file.

- **ITMAX** : maximum allowable number of iterations in the head solution (ADIP)
  - Normal range : 100 - 200 (according to user's manual)
  - Default = none

- **NREC** : number of pumping or injection wells to be specified in Data Set # 2. The program treats wells differently than diffuse sources.
  - If NREC = 0, the program will NOT attempt to read Data Set # 2 which should be omitted
  - Default value = 0
  - Minimum value = 0
  - Maximum value = 10 (or appropriate arrays must be redimensioned.)

- **NPTPND** : initial number of particles per block (node)
  - Allowable values : 4, 5, 8, 9
    - Allowable values are limited by geometric symmetry requirements
    - An allowable value must have enabling logic coded into the program in subroutine GENPT
    - A supplement from USGS gives coding and instructions to add a 16 particle-per-block option to the program (It has not been implemented in our version, because CYBER storage limitations would be exceeded in the Otis simulation.)
    - Default value = none

- **NCODES** : number of different node identification codes to be specified in Data Set # 6
  - Minimum value = 0 (no codes are required if no diffuse, vertical flow (as in leakage or recharge) is present
  - Wells are NOT considered diffuse vertical flow, and the well I/O is handled separately in the code.
  - Default value = 0 (no cell-wide recharge or leakance)
  - NO upper limit specified in program
    - BUT, relevant COMMON (dimensioning) statements in source code must be revised if NCODES > 10
    - Simulation of Otis A.N.G.B. required NCODES = 6

- **NPNTMV** : particle movement interval for printing chemical output data
  - Default value = 0 (print at the end of each time step)
  - Program automatically prints data every 50 moves

- **NPNTVL** : option for printing computed velocities
  - 0 = never [default]
  - 1 = after first step only
  - 2 = after all steps
  - >=3 is treated as 0

- **NPNTD** : option for printing computed dispersion equation coeff's
  - 0 = never [default]
  - 1 = after first time step only
  - 2 = after all steps
  - >=3 is treated as 0

- **NPDELC** : option for printing computed changes in concentration
  - 0 = no print [default]
  - 1 = print
  - any other values treated as NPDELC = 1

CARD # 3 Real Parameters (Aquifer-wide) :

PINT		POROS		S		TINIT		YDEL		CELDIS	
	TOL		BETA		TIMX		XDEL		DLTRAT		ANFCTR
G5	G5	G5	G5	G5	G5	G5	G5	G5	G5	G5	G5

- **General :**

- **PINT** : Pumping Period [years] (total time simulated)
  - Default = none
  - Minimum = none
  - Maximum = none

- **TOL** : Convergence Criterion (Tolerance) in ADIP [FT]
  - Definition :
    - during each iteration, the subroutine ITERAT finds the cell with the greatest change in head [FEET]
    - to achieve convergence, that change may not exceed TOL
  - Default = **none** (the run cannot converge).
  - Usual range = 0.0001' to 0.001'

- **POROS** : Effective Porosity of aquifer [decimal fraction]
  - Default = **none** (program will abend)
  - Common Values of actual porosity :
    - unconsolidated sand : 0.25 - 0.50
    - sandstone : 0.05 - 0.30
    - shale : 0.00 - 0.10
    - * if porosity (excluding fractures) is too low, as in some fractured rocks, more groundwater flows through the fractures than through the pores.

- **BETA** : Characteristic dispersion length [feet]
  - Default = 0.00 No dispersion
  - Minimum = 0.00 No dispersion
  - Maximum = (set by block size considerations)
  - BETA Values can be set by :
    - the largest common particle size in the aquifer (generally, other factors override this)
    - the size of the largest inhomogeneities
    - the characteristic distance between inhomogeneities in aquifer
    - empirical considerations : use the value needed to fit the data
  - Some numerical dispersion built in to the method of characteristics. This numerical dispersion might allow a user to input an artificially low value for BETA.
    (apparent dispersivity) = BETA + (numerical dispersivity)
  - General advice from Dr. Voss :
    - XDEL (or YDEL) <= 4.0 * BETA

- S : Storage Coefficient
  - For steady-state flow conditions set S = 0
  - For unsteady-state flow conditions :
    - Default value = **0.0** = minimum value
    - for WATER TABLE conditions, S = either :
      - the porosity or
      - the net free drainage
    - for Artesian conditions : pressure-induced storage, and would tend to involve changes in matrix porosity due to changes with pressure.
    - currently **NO** provision S to enter cell-by-cell data.

. **TIMX** : Time Increment Multiplier for transient flow problems.
  . Steady-state flow problems :
    . Use Default value = **0.0** = minimum value
    . TIMX is Set = 0 automatically if S = 0.0
  . Unsteady-state flow problems :
    . Use a value >= 1.0 to :
      . enhance algorithm stability
      . improve efficiency

. **TINIT**: Size of initial time step [seconds].
  . Steady-state flow problems :
    . TINIT is disregarded if S = 0.0
    . Use Default value = 0.0
  . Unsteady-state flow problems :
    . Enter the appropriate value (> 0)

. **XDEL** : Width of a finite difference cell in X direction [ft]
  . Limited by :
    . significance and precision of input data
    . geography & topography of aquifer
    . level of detail required in results
    . variability of physical properties of aquifer
    . program's built-in stability criteria (see User's Manual, pp 11 - 13)
    . core and disk storage capacities of computer system
    . relationship of XDEL to BETA :
      . solute plume problems $X \leq 4 * BETA$
        (from Dr. C. Voss concerning SUTRA)
  . No default : run abends

. **YDEL** : Width of finite difference cell in Y direction [ft]
. Limited by :
    . same factors as XDEL
. No default : run abends

. **DLTRAT** : Ratio of transverse to longitudinal dispersivity
  . commonly varies from 0.1 to 0.5
  . most common value is about 0.3
  . allowable values = 0.00 to 1.0
  . default value = **0.00**

. **CELDIS** : maximum distance travelled per particle move by the fastest moving particle
  . this is part of to algorithm's automatic, built-in stability criteria
  . [expressed as a decimal fraction of XDEL and YDEL]
  . allowable values are 0.00 to 1.00
  . shorter distances require more computer time
  . longer distances are less accurate, as a particle's stream (flow) line diverges from its straight-line extrapolation.

. **ANFCTR** : Ratio of T(yy) to T(xx) -- anisotropy of transmissivity
  . possible range : 0.0 to 1.00 to infinity
  . default value = none
  . usual value = 1.00 (isotropic)
  . logical value for a level, unconsolidated sand-and-gravel aquifer = 1.0

Optional Card That Would Be Used Only For Augmented Version With Chemical Reaction, Radioactive Decay & Adsorption As Prepared by J. V. Tracy of Ertec Western, Inc. for U.S. Nuclear Regulatory Commission

NDECAY		DCYTIM		SORBQR		SORBAL
	NSORB		DENROCK		SORBST	
I5	I5	F10.5	F10.5	F10.5	F10.5	F10.5

. **NDECAY** :
  . If NDECAY = 0 NO decay will be simulated.
  . If NDECAY = 1 decay WILL be simulated.

. **NSORB** :
  . If NSORB = 0 NO adsorption will be simulated
  . If NSORB = 1 adsorption simulated : linear isotherm
  . If NSORB = 2 adsorption simulated : Langmuir isotherm
  . If NSORB = 3 adsorption simulated : Freundlich isotherm

. **DCYTIM** :
  . If NDCAY = 0, program sets DCTIM = 0
  . If NDCAY = 1, program reads DCTIM, and treats it as a half-life

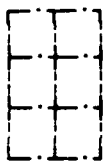
. **DENROCK** : specific gravity of aquifer rock
  . if NSORB = 0, DENROCK = 0.
  . if NSORB = 1,2,3 program reads DENROCK, treats it as specific gravity of aquifer

. **SORBQR** : adsorption coefficient
  . if NSORB = 0, SORBQR = 0.0
  . if NSORB = 1,2,3 SORBQR = Kd in ml/g

. **SORBST** : sorption saturation value for Langmuir solver
  . if NSORB = 2 SORBST = sorption saturation value
  . if NSORB = 0,1,3 SORBST = 0.0

. **SORBAL** : exponent in the Freundlich isotherm
  . if NSORB = 3 SORBAL = alpha
  . if NSORB = 0,1,2 SORBAL = 0.0

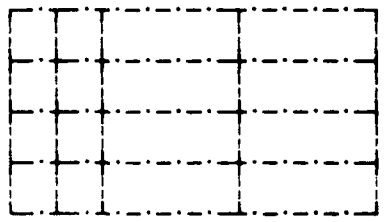
DATA SET # 1 : Locations of observation points.



IXOBS IYOBS
I2 I2

- Number of Observation Points : **NUMOBS** (on Card # 2)
- Sets number of data cards in this data set
- Zero to five observation points are allowed.
  - (COMMON statements in source code can probably be revised to allow more observation points if necessary)
  - No observation points are required
- IF no observation points are desired :
  - NUMOBS = 0 on Card # 2
  - DELETE this data set
- OTHERWISE, for each observation point, need a card with a pair of X-Y coordinates
  - IXOBS . IYOBS

DATA SET # 2 : Pumping / Injection Well Data
(First pumpage period)



IX IY REC CNRECH
I2 I2 F8.2 F8.2

- Number of pumping / injection wells : **NREC** : (on Card # 2)
  - May have up to NX x NY wells (1 per cell)
  - Limit of 1 well per cell
    - if any cells have more than one well :
      - algebraically add the flow rates, and treat as one well
  - No wells are required in any cell, or in the whole aquifer
  - IF NO wells are desired :
    - NREC = 0 (on Card # 2)
    - delete DATA SET # 2
  - Pumpage rates MAY change with time. Handle by specifying multiple pumpage periods. (Pumping rates are constant within each period.)

- Data for the first pumpage period are specified in this data set
- Data for any subsequent pumpage periods would be specified in Data Set # 10 C

- IF well data ARE desired , enter the data here for the first pumpage rate period :
  - one card per well, each with :
    - IX = X coordinate of well
    - IY = Y coordinate of well
    - REC = pumping rate of well in [cubic feet/sec]
      - (+) = pumping
      - (-) = injection
    - CNRECH = concentration of recharge flow [ppm]
      - for pumpout wells, CNRECH = the current conc in that cell

- Leakage and recharge can be simulated as either point sources/sinks (wells), or distributed (cell-wide) leakage/recharge.
  - These flows can often be simulated as either cell-wide flows or as point (well) flows. The user has only to choose one or the other, and to keep the coefficients consistent.

  - The program includes an internal logic to avoid singularity problems near wells. (This logic is unnecessary for and NOT used for distributed flows.)
    The program also creates and destroys particles, as necessary, at wells, but NOT at diffuse sources/sinks.

  - Point/well flows are specified here (in Data Set # 2). and are stored in the array REC(i,j)
    Cell-wide leakages/recharges are specified in Data Sets # 5 and # 7, and rates are stored in the array RECH(i,j)

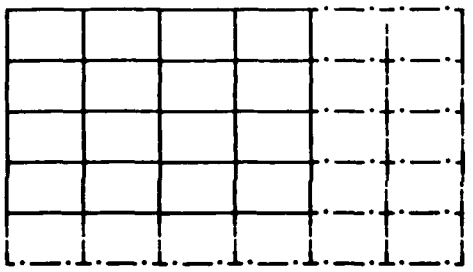
DATA SET # 3 : Parameter Card/Map for Transmissivity :

- Program has provisions for inputting spatially constant transmissivities, or for varying transmissivities as block-wise parameter maps.
- The program does NOT have provisions for transmissivity or permeability to change with time, or for transmissivity to change with with saturated thickness.
- The outermost rows and columns of blocks are set to zero transmissivity (and permeability) to simulate the imaginary impermeable boundary, which is assumed by the model
- Constant transmissivity case :
  - the transmissivity is constant across the aquifer (except for the outermost rows and columns of blocks, which are automatically set impermeable by the program).
- Non-constant transmissivity case :
  - the user inputs a map of transmissivity values, blockwise.
  - for each block, the program multiplies FCTR by VPRM(i,j) and stores each product in the array VPRM(i,j)

- Internal handling of this data :
  - Read in by subroutine PARLOD.
  - Initially stored in the array VPRM(I,J).
  - Harmonic mean transmissivities, TRMX(i,j,1) and TRMX(i,j,2), are calculated and stored for each cell in subroutine PARLOD.
  - Cellwise permeability values are calculated in PARLOD from the cellwise transmissivity and thickness values.
  - The array, VPRM(I,J) is then zeroed out, and thus freed up for use with vertical permeability data in Data Sets # 6 and #7.

CELL SATURATED THICKNESS :

INPUT	FCTR
I1	G10.0



VPRM(1,y)	VPRM(3,y)	VPRM(5,y)
VPRM(2,y)	VPRM(4,y)	VPRM(6,y)
G4.1 G4.1	G4.1 G4.1	G4.1 G4.1

- First Card :
  - INPUT = 1 (for non-constant transmissivity)
    0 (for constant transmissivity)
  - FCTR = transmissivity factor/value

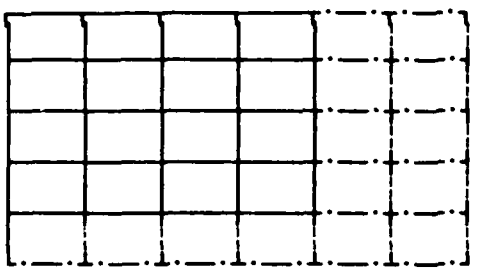
- Subsequent Cards (NY * N) (N an integer)
  - each card contains the transmissivity multiplier, VPRM(I,J) for each column in its row
  - may need more than one card per row if more than 80 (or 136) spaces per row are required.
    - (N cards per row of cells).
- In the outermost rows and columns, VPRM(I,J) = 0.0
  - To avoid confusion, the user can do this in the input file.
  - Just in case, this is done automatically by the program in subroutine PARLOD
- Limits on the size of the array were discussed in NX and NY on Card # 2. The USGS source code is written for arrays dimensioned at a maximum of 20 x 20 cells.
  - for smaller arrays, the source code can be used as is.

- for larger arrays, the dimension statements must be modified in the main program and all relevant subroutines.
- the program is still under constraint of the operating system size limitations.

DATA SET # 4 : Aquifer Thickness Data

- The user must input data for a thickness value [in feet] for each block in the aquifer.
- The program, as written, does NOT contain logic to vary the cell thicknesses with time.
- If the cell thicknesses DO change over time, one must :
  - use time-average values.
  - make separate simulation runs over successive time periods as the thicknesses change.
  - modify the source code to adjust the thicknesses over time.
- Thickness data can be entered as an array-map
- This data is stored in array THCK(I,J)
- The current source code CANNOT support a one-line input of a constant value of aquifer thickness for all cells, because :
  - code must be added to specify zero thickness for all cells with zero transmissivity (especially the boundary cells)
  - the program logic assumes that the thickness of each impermeable cell (such as each cell along the outer boundary) must have zero thickness.
  - if this is NOT done, the as-written program will abend, without giving adequate diagnostics.
- User options include :
  - always specifying a thickness map, with zero thickness at all boundaries, and at all other impermeable cells
  - add a loop to the source code in PARLOD to automatically zero the thicknesses of all impermeable and boundary cells.
  - add diagnostic warnings to warn the user before the run bombs due to improperly specified cell thicknesses.
- So, the user will enter :
  - FCTR : a constant by which all cellwise entries are multiplied.
  - THCK(i,j) : a relative thickness value for each cell
- In the current program, for each cell, the program will :
  - multiply FCTR * THCK(i,j)
  - store the result in THCK(i,j)

INPUT	FCTR
I1	G10.0



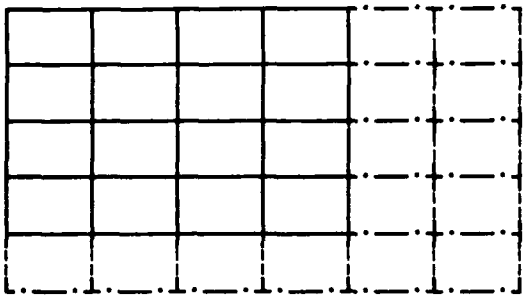
THCK(1,y) THCK(3,y) THCK(5,y)
THCK(2,y) THCK(4,y) THCK(6,y)
G4.1 G.1 G4.1 G4.1 G4.1 G4.1

- Card # 1 : INPUT = 1
  FCTR = _____
- Remaining Cards (N*NY) :
  Enter the aquifer thickness map :
  - for each cell, enter a multiplier factor so that :
    THCK(i,j) = FCTR * THCK(i,j)

DATA SET # 5 : Recharge Rate Data_

- Comments :
  - this data is for :
    - diffuse (cell-wide) recharge (or leakage) in the vertical direction
    - point sources/sinks are specified separately as wells (in Data Set # 2)
  - if the rate is spatially uniform for the whole aquifer, only one line of data is required.
  - the program, as written, cannot simulate diffuse recharge/ leakage that changes with time. Options are :
    - choose time-averaged values
    - simulate these flows as point sources, which CAN vary with time
    - modify the source code (a non-trivial undertaking)
  - this data set canNOT be omitted, but can be specified with one card at a uniformly zero rate (a quasi-default value).

INPUT FCTR
I1 G10.0



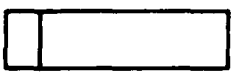
RECH(1,y) RECH(3,y) RECH(5,y)
RECH(2,y) RECH(4,y) RECH(6,y)
G4.1 G4.1 G4.1

- Specification of Spatially uniform rates :
  - only one card is required, with two data fields:
    - INPUT = 0 [dimensionless]
    - FCTR = ____ [ft/sec]

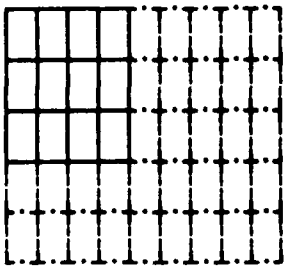
- Specification of spatially nonuniform rates :
  - first card : two data fields :
    - INPUT = 1 [dimensionless]
    - FCTR = ____ [ft/sec]
      (this value is non-final, and is multiplied by RECH(I,J) for each cell)
  - subsequent cards (NY)
    - one card per row of cells (format permitting)
      - two or more lines per row if format requires > 80 char/line
    - each RECH(i,j) is a multiplier applied to FCTR
    - each product is then stored in RECH(i,j)

DATA SET # 6 : NODE ID DATA :

- Comments :
  - Often, a simulated aquifer will contain a large number of blocks, but only a small number of frequently repeated diffuse leakage/ recharge boundary conditions.
  - This command permits a user to conveniently assign repetitive boundary conditions to a large number of blocks.
  - The user lists the types of cell boundary conditions in Data Set # 7.
  - Here, the user creates a map, NY rows by NX columns
    - Normally, each line of data contains NX fields of I1 data (Must use I2 format if NCODES > 9)
    - Each field contains the NODEID of a cell in the aquifer.
  - ICODE = 0 is always available for cells without diffuse leakage
  - This data set canNOT be entirely omitted.
    At minimum, enter values of 0, 0 on the first card



INPUT FCTR
I1 G10.1

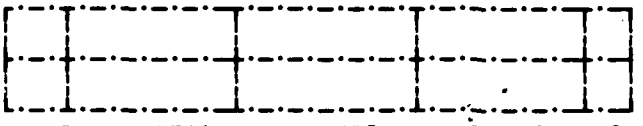


NODEID(i,j), (i = 1, NX)
format (NYI1)

. Input Data :
  . First Card :
    INPUT = 1
    FCTR = 1
  . Subsequent Cards (NY)
    NODEID(i,j), (i= 1) (0 <= NODEID(i,j) <= NCODES)
    see DATA SET # 7 for permissible values of NODEID

DATA SET # 7 : Definitions of cell boundary condition 'types'

. Number of Cards required = NCODES (see Card # 2)
  . minimum value = 0 (No diffuse vertical leakage (or recharge) is present. Injection and pumpout wells do NOT require codes.)
. If NO cells have diffuse vertical flow boundary conditions :
  . must include one card in this data set with values for a specified but unused cell type.



ICODE	FCTR1	FCTR2	FCTR3	I2
I2	G10.2	G10.2	G10.2	OVERRD

. For each different cell ID code, the following information must be specified :
  . ICODE : the code number for this cell 'type'
  . FCTR1 = leakance coeff (vertical) = K'/b [1/sec]
    where :
    . K' = the permeability of a horizontal confining layer to vertical leakage into or out of a cell [ft/sec]
    . b = the thickness of the horizontal confining layer [ft]
  . FCTR2 = solute concentration in recharge fluid [ppm] applies only to in-flow, (overridden for out-flow)

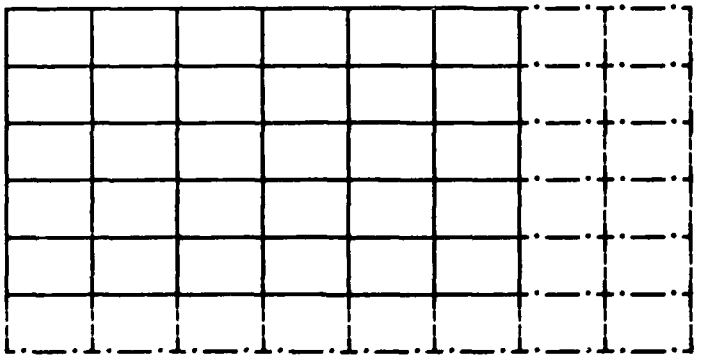
- FCTR3 = recharge rate [ft/sec]
  - used if the OVERRD switch = 1. The value of RECH(I,J) previously specified in Data Set # 5 will be replaced by FCTR3.
  - ignored if the OVERRD switch = 0. The value of RECH(I,J) previously specified in Data Set # 5 will be retained.
- OVERRD = override switch. (just explained).

DATA SET # 8 : Initial/Boundary Value Water Table Data

Comments :

- A value is needed for each cell in the grid, but may be supplied by default coding (including a blank card in the deck).
- These values are treated as initial conditions for each cell
- These values are ALSO treated as boundary values for each cell with a non-zero diffuse leakage/recharge specification.
- If this w.t. value is the same for all cells, a simplified data set can be used, requiring only one card with two inputs.
- If there is any initial variation in the w.t. values, a complete map of the initial aquifer water table must specified.
- If this data set is totally omitted, an execution-time read error will probably result.
- If one blank card is used for this deck, the water table will be initialized at 0' elevation (at the reference elevation) in all cells.

INPUT	FCTR
I1	G10.0



WT(1,y)	WT(3,y)	WT(5,y)	WT(7,y)
WT(2,y)	WT(4,y)	WT(6,y)	WT(8,y)
G4.1	G4.1	G4.1	G4.1

Input Parameters :
. First Card :
  . all cells identical :
    . INPUT = 0 . FCTR = WT
  . all cells initially 0. :
    . one blank card acts as the data set
  . some cells different :
    . INPUT = 1 . FCTR = 1.000
. Remaining Cards :
  . all cells identical : omit
  . some cells different :
    . enter a 2-D array, NY rows x NX columns

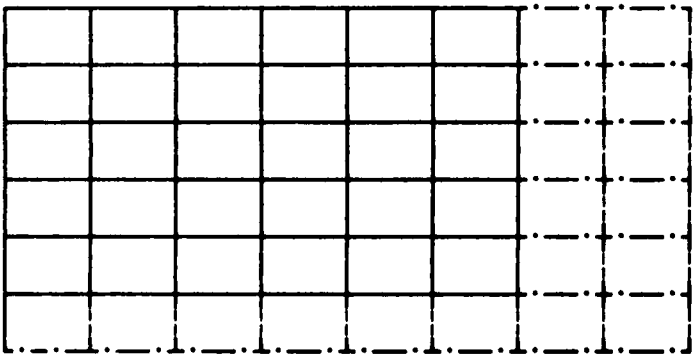
DATA SET # 9 : Initial Groundwater Concentration by Cell

Comments :

. the program reads in the initial concentration value for each cell
. this data set is mandatory
. if this data set is totally omitted, an execution-time read error may occur
. if one blank line is used, the program will initialize all cells at zero concentration.
. the program treats the concentration units as ppm
. NO blank lines are inserted BETWEEN or after any lines in this data set

Input Parameters :

INPUT FCTR
I1 G10.0



CONC(1,y) CONC(3,y) CONC(5,y) CONC(7,y)
CONC(2,y) CONC(4,y) CONC(6,y) CONC(8,y)
G4.1 G4.1 G4.1 G4.1

INPUTS :
. if the initial concentration is the same in all cells,
  see comments above
. otherwise :
  . INPUT = 1 FCTR = 1.00 (or another appropriate real value)
  . enter CONC(i,j) in PPM
  . the G4.1 format can be changed in the source code, when necessary

DATA SET # 10 : Data for Multiple Groundwater Flow Time Periods :
. Comments :
  . When only one such time period is required (for steady-state groundwater flows) this data set consists of one blank card. Omission of this blank card will cause an execution-time read error.
  . Otherwise, the following inputs can be revised each subsequent period :

. NTIM	. NPNT	. NITP	. ITMAX	. NREC
. NPNTMV	. NPNTVL	. NPNTD	. NPDELC	. NPNCHV
. PINT	. TIMX	. TINIT	. REC(x,y)	. CNRECH(x,y)

  . Any other data cannot be changed over time. The user's options are :
    . neglect changes that would have insignificant effects
    . use time-average values when possible
    . make a separate simulation run for each time period

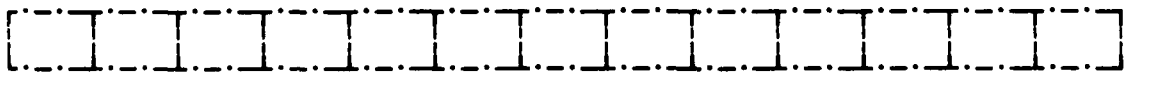
  . Data Set # 10 has three sections :

    . Card A :

ICHK
I1

      . ICHK = switch :
        . ICHK = 0 : NO data to be revised
        . ICHK = 1 : data to be revised

      . Card B :



NTIM		NITP		NREC		NPNTVL		NPDELC		PINT		TINIT
	NPNT		ITMAX		NPNTMV		NPNTD		NPNCHV		TIMX	
I4	I4	I4	I4	I4	I4	I4	I4	I4	I4	G5.0	G5.0	G5.0

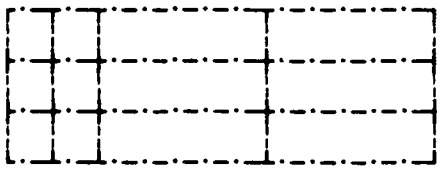
      . see Cards # 2 and 3 for further information :

      . **NTIM** : number of time steps per pumping period.

- **NPNT** : time step interval for printing hydraulic and chemical output data
- **NITP** : number of iteration parameters
- **ITMAX** : maximum allowable number of iterations in the head solution (ADIP)
- **NREC** : number of pumping or injection wells to be specified in Data Set # 2
- **NPNTMV** : particle movement interval for printing chemical output data
- **NPNTVL** : option for printing computed velocities
- **NPNTD** : option for printing computed dispersion equation coeff's
- **NPDELC** : option for printing computed changes in concentration
- **PINT** : pumping period (years) (total)
- **TIMX** : Time increment multiplier for transient flow problems.
- **TINIT** : Size of initial time step [seconds].

. Card 10 C (# 1 - NPUMP)

. Revised Pumping Data for this Pumping (Time) Period :



IX IY REC CNRECH

(One card per well)

- IX = X coordinate of well
- IY = Y coordinate of well
- REC(i,j) = flow rate of well
- CNRECH(i,j) = concentration of flow from well

  (for flow from well, program assumes the current concentration of the cell)

. Structure of a Data Set # 10 :

```
   .  Card A : ICHK = 1  (for time period # 2)
      Card B :   **      ( "    "    "    # 2)
      Card C :   ***     ( "    "    "    # 2)
      Card A : ICHK = 1  ( "    "    "    # 3)
      ..........................................
      ..........................................
      Card A   ICHK = 1  ( "    "    "    # NSTEP)
      Card B     **      ( "    "    "    # NSTEP)
      Card C     ***     ( "    "    "    # NSTEP)
      Card A   ICHK = 0  (no more time periods)

       **  enter the data appropriate for Card B
      ***  enter the data appropriate for Card C's
```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APPENDIX D. USGS-2D BASE CASE INPUT DATA FILE FOR THE OTIS SEWAGE PLUME

```
KONIKOW   OTIS   WHKOTSA   OLD BASE CASE   K= 194   TILT B
  10   1  36  40 7500   1   7   2 100   0   5   6   0   1   0   0   0
  40..0001  .35  40.   0.              500. 750.  0.3 0.50  1.0
915
1820
1  4.520D-3
   0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
   0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.
   0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0. 77. 77. 77. 77. 77.
  77. 77. 77. 77. 77. 77. 77. 77. 77. 77.  0.  0.  0.  0.  0.  0.
   0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0. 75. 75. 75. 75. 75.
  75. 75. 75. 75. 75. 75. 75. 75. 75. 75. 75.  0.  0.  0.  0.  0.
   0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0. 73. 73. 73. 73. 73. 73.
  73. 73. 73. 73. 73. 73. 73. 73. 73. 73. 73. 73.  0.  0.  0.  0.
   0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0. 71. 71. 71. 71. 71. 71. 71.
  71. 71. 71. 71. 71. 71. 71. 71. 71. 71. 71. 71.  0.  0.  0.  0.
   0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0. 69. 69. 69. 69. 69. 69. 69.
  69. 69. 69. 69. 69. 69. 69. 69. 69. 69. 69. 69. 69.  0.  0.  0.
   0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0. 67. 67. 67. 67. 67. 67. 67. 67.
  67. 67. 67. 67. 67. 67. 67. 67. 67. 67. 67. 67. 67.  0.  0.  0.
   0.  0.  0.  0.  0.  0.  0.  0.  0.  0.  0. 65. 65. 65. 65. 65. 65. 65. 65. 65.
  65. 65. 65. 65. 65. 65. 65. 65. 65. 65. 65. 65. 65.  0.  0.  0.
   0.  0.  0.  0.  0.  0.  0.  0.  0.  0. 63. 63. 63. 63. 63. 63. 63. 63. 63. 63.
  63. 63. 63. 63. 63. 63. 63. 63. 63. 63. 63. 63. 63. 63.  0.  0.
   0.  0.  0.  0.  0.  0.  0.  0.  0. 61. 61. 61. 61. 61. 61. 61. 61. 61. 61. 61.
  61. 61. 61. 61. 61. 61. 61. 61. 61. 61. 61. 61. 61. 61.  0.  0.
   0.  0.  0.  0.  0.  0.  0.  0. 59. 59. 59. 59. 59. 59. 59. 59. 59. 59. 59. 59.
  59. 59. 59. 59. 59. 59. 59. 59. 59. 59. 59. 59. 59. 59. 59.  0.
   0.  0.  0.  0.  0.  0.  0. 57. 57. 57. 57. 57. 57. 57. 57. 57. 57. 57. 57. 57.
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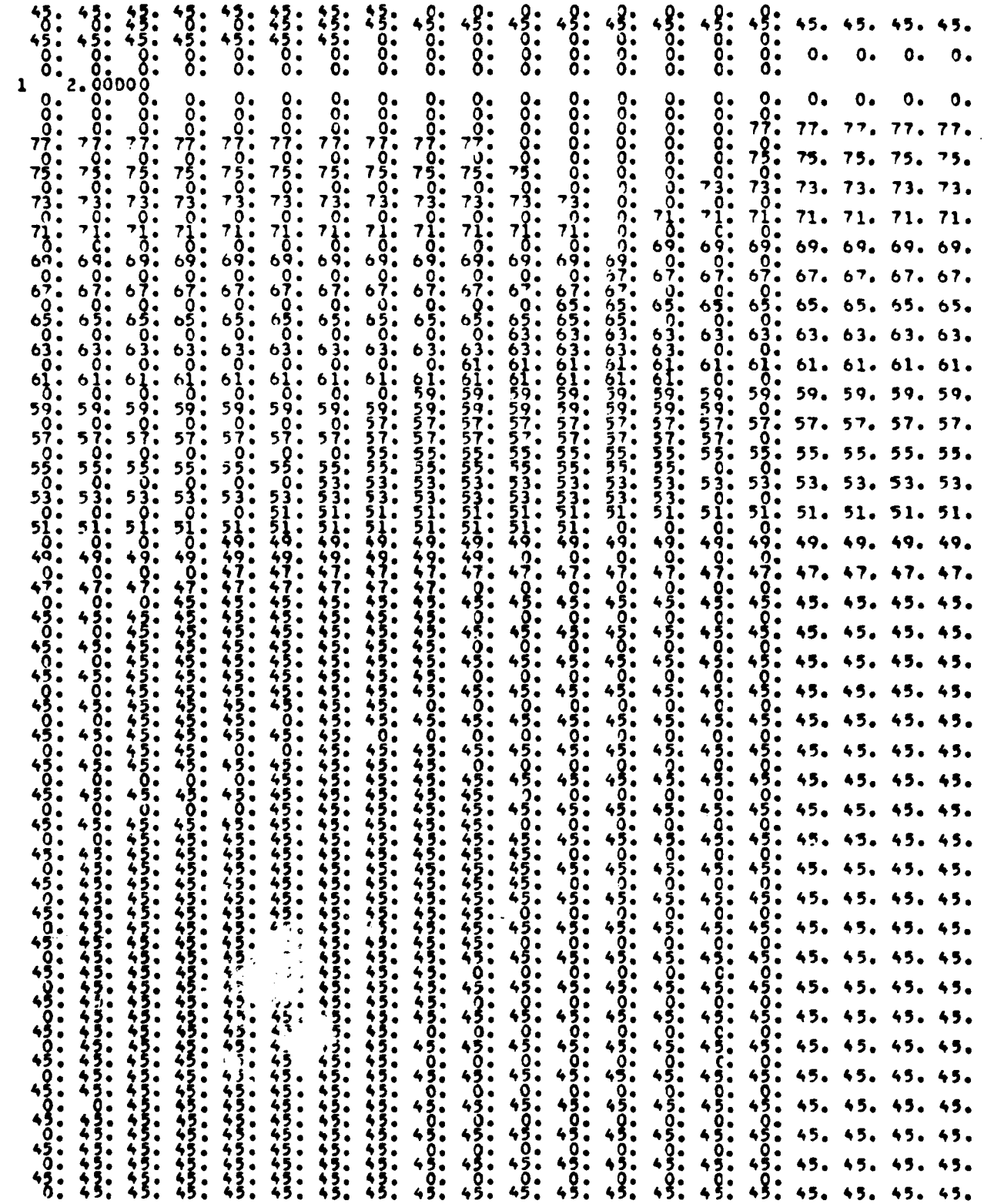

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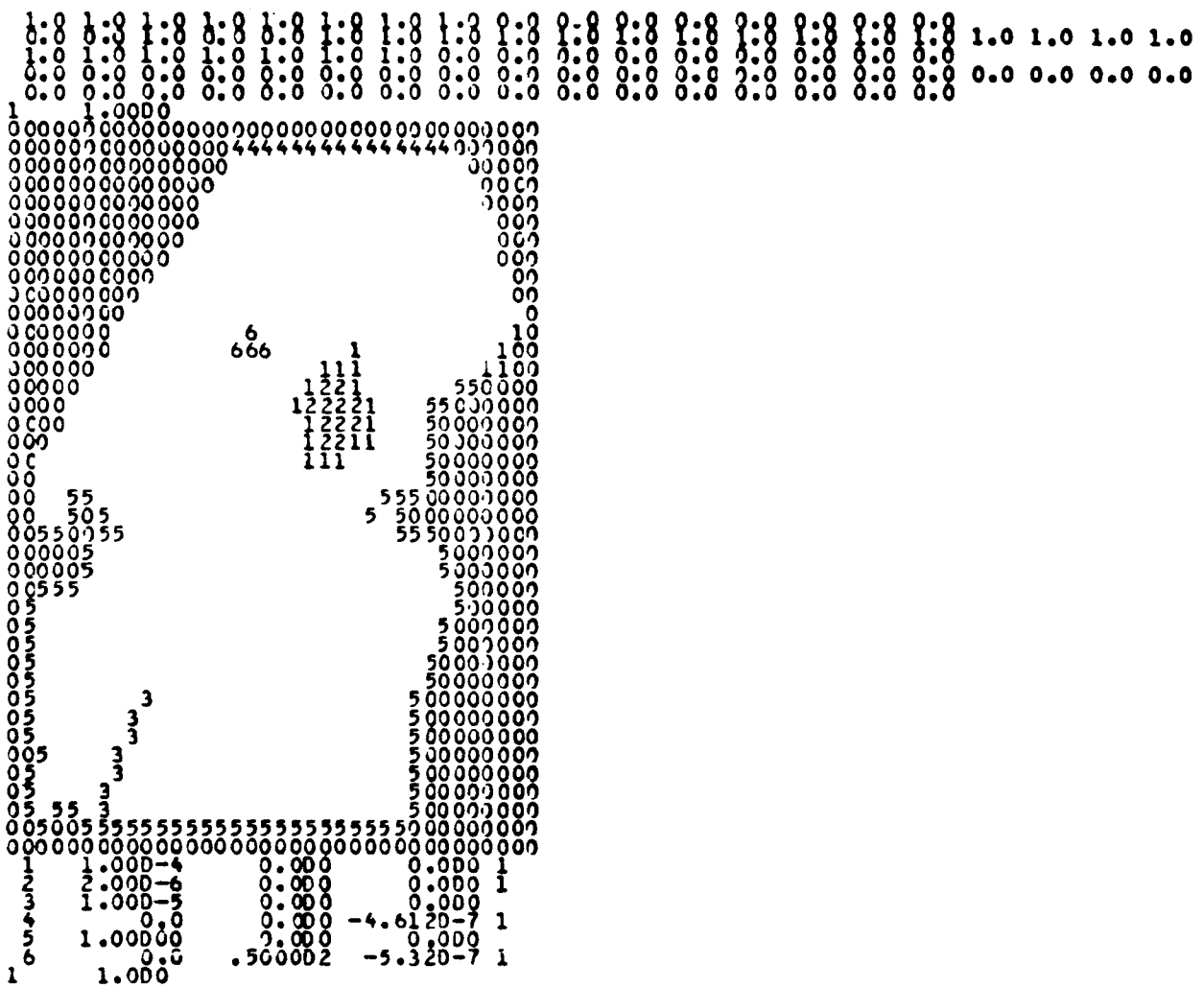
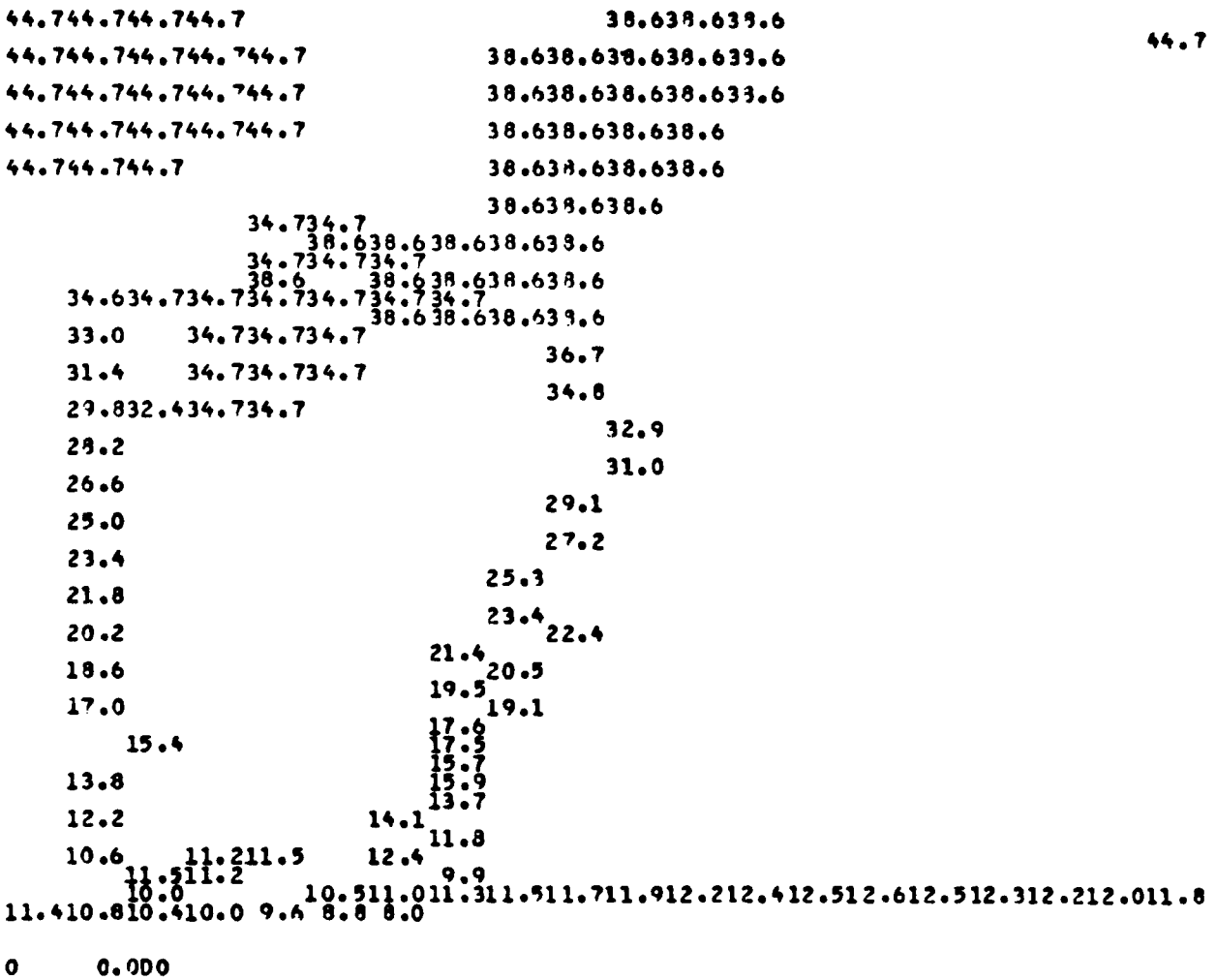


38.6

44.7 38.6

44.744.744.7 39.638.6



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APPENDIX E

ANNOTATED INPUT DATA FILE TEMPLATE
ILLINOIS RANDOM WALK PROGRAM

****

NOTES :
The program was originally written for punched card input. It is currently being used with interactive terminal input. So, where the term "card" is used, the word "line" can generally be substituted.

Empty brackets in the units column (at the right) signify that the parameter is dimensionless. [ ]

Several versions of the program exist in the RDVDYN1 library. The variables are the same, but formats may differ slightly, and any format error will cause a run to abend. Before preparing your file, get a printed listing of the exact version of the source code, and adjust the input parameter formats on this template.
Values of some variables depend on values of other variables defined on following cards. Check the following cards if previously undefined variables are encountered.

TITLE CARD :

TITLE

Sufficient information to identify the run.

13A10

TITLE = Up to 130 alphanumeric characters used to identify the simulation run and its key input parameter values

[SS = steady-state groundwater flow solution, usually with a moving concentration plume]
[USS = unsteady-state ground water flow solution]

PARAMETER CARD

NSTEPS	DELTA	ERROR	NPITS
1	.1E11	.1E0	40
I6	E6.0	E6.0	I6

NSTEPS = total number of time increments in groundwater flow solution [ ](1)
= NSP x NRT

[SS] NSTEPS = 1
default value = 0 (works the same as 1)
[USS] NSTEPS = NSP X NRT (as appropriate)
default value : 0 : [unsatisfactory for USS simulation]

DELTA = [SS] : 1.0E10 [days]
default value : 0 [program will abend]
(The users manual recommends 1.0E10. A large value (such as 40 years (1.46E4 days for Otis) may work about as well.
[USS] : 1/6 of the time increment for significant drawdown to occur
default value : none [program will abend]

ERROR = [SS] 0.10 (or more if it works OK) [ft]
[USS] : [ft]
. initial value = Q x DELTA / (10 x DELX x DELY x 7.48 x S)
. adjust value downward until program results are unaffected
. default value : none [program will abend]

NPITS = number of times that the particles will be advanced per groundwater flow period [ ]
[SS] as required
[USS] as required :
. NPITS x DELP = length of time of simulation
. can increase DELP [and increase NPITS correspondingly] until the solution ceases to change, or until the computer run time becomes excessive.
. But, changing DELMAXX is more efficient. DELMAX is explained in the report, Sections III and VII.
. if NPITS too large, : CPU time & printout volume expensive

(1) [ ] signifies a dimensionless parameter.

. if NPITS too small, : extrapolation errors may
  creep into calculations of particle locations
. default value : 0 [treated as NPITS = 1]

DEFAULT VALUE CARD

NC	NR	TT	S1	HH	QQ	RR	RRH	RRD	S2	CCH
24	16	.125E6	.13E-3	.40E2	-.1E-5	0.0E0	4.3E1	-1.0E1	.30E0	.15E2
I8	I8	E8.2	E8.2	E8.2	E8.2	E8.2	E8.2	E8.2	E8.2	E8.2

PP	BOTT
.138E4	-.14E3
E8.2	E8.2

(All values except NC and NR would be overridden for specific cells
 by any corresponding values on node cards)

NC = number of columns of nodes in grid (NX) [ ]
NR = number of rows of nodes in grid (NY) [ ]
- . if NC [or NR] is too small, discretization errors occur
- . in 1-D simulations, the grid may be two nodes (1 cell) wide
- . rule of thumb for plume simulation :
  DELX <= 4 * DISPL
- . if NC [or NR] is too large :
  - . CPU time and elapsed run time increase
  - . computer core memory availability may be exceeded.
- . the default values won't function properly

TT = default aquifer transmissivity [gal/day/ft]
- . this default value is used for both the X and Y dimensions
- . the node deck and the built-in calculations handle Txx and Tyy separately.
- . during program execution :
  - . cell transmissivity will be taken from the default card or node cards on the first iteration.

. in subsequent iterations, transmissivity is calculated as (hydraulic conductivity) * (saturated thickness)

S1 = default storage factor for Artesian aquifer conditions [gal]
(reflects changes in aquifer porosity with pressure.)

HH = default cell heads : initial conditions [ft]

QQ = default leakage (+) / recharge (-) rate [gal/day-cell]
(this value represents only distributed sources)
. Pump rate data and distributed flow source/sink data are entered separately. The program will automatically merge these two data sets during the run.
. QQ values are head-independent
. QQ would be useful as a net rainfall or evaporation rate

RR = default recharge factor [gal/day/ft]
. this is effectively a leakance value
. it pertains to head-dependent sources/sinks
. rate = R * (RRH - H)

RRH = default elevation of land or pond surface [ft]
(pond surface elevations at Otis were handled on individual node cards)
. helps determine rate and direction of recharge/leakage flow
. in the model, this is a boundary condition for an artesian aquifer cell

RRD = default elevation : [ft]
. of bottom of pond bed OR
. below which evapotranspiration ceases
(in Otis simulations elevation of pond bottoms were handled on individual node cards)
. a boundary condition value

S2 = default storage factor for "water table" aquifer [gal/ft]
similar to porosity

CCH = default elevation for top of aquifer [ft]

PP = default hydraulic conductivity for aquifer boundary conditions. During program calculations, permeability and saturated thickness are used in updating transmissivity values. [gal/day/ft²]

BOTT = elevation of bottom of aquifer [ft]

PUMP PARAMETER CARD

NPUMP	NSP	NRT
19	2	1
I6	I6	I6

NPUMP = number of pumps in system
- minimum = 0 = default
- maximum = 100 [unless 3 arrays in source code are redimensioned.]

NSP = number of time increments per pumpage period
- default = 0 [program abends]
- minimum = 1
- typical value = 2 [1 or 2 work equally well on Otis steady-state simulation]

NRT = number of pumpage periods
- minimum = 1 = steady-state
- default = 0 [program abends]

PUMPING SCHEDULE CARDS

IP	JP	P1	P2	P3	P4
2	16	1.22E5			
2	17	1.22E5			
2	18	1.22E5			
I3	I3	E6.0	E6.0	E6.0	E6.0

IP = X coordinate of node associated with the well [ ]
JP = Y coordinate of node associated with the well [ ]
- limited to 100 wells, unless the three affected arrays in the source code are redimensioned.
- there can be only 0 or 1 well per node

P1 = pumping rate : Period 1 [gal/day]
- pump 1 must always be specified, due to the FORTRAN 4 DO Loop. The rate can be 0.

P2 = pumping rate : Period 2 (+) = withdrawal [gal/day]
P3 = " " : Period 3 (-) = recharge [gal/day]
P4 = " " Period 4 [gal/day]

- when blank rate fields are read, they are read as 0.00
- because this program is written in FORTRAN IV, at least one card must always be included in this pumping rate data deck.
- The program will always make at least one pass through the data reading DO Loop, even when NPUMP = 0.
- When there are no pumps, this card will contain dummy data :

  0 <= IP <= NX 0 <= JP <= NY P = 0.0

VARIABLE GRID CARD(s) -- DELX

DELX(1)	DELX(2)	DELX(3)	DELX(4)	DELX(5)	DELX(6)	DELX(7)	DELX(8)
500.	500.	500.	500.	500.	500.	500.	500.
500.	500.	500.	500.	500.	500.	500.	500.
500.	500.	500.					
F8.0	F8.0	F8.0	F8.0	F8.0	F8.0	F8.0	F8.0

ITERATION CONTROL DATA

8

1	1.E-5	1.E-5
ITRMAX	RPMAX	RUMAX
I10	D10.0	D10.0

ITRMAX = Maximum number of iterations/step. [ ]
1 = non-iterative solution
RPMAX = Abs. convergence criterion (head) [meters]
RUMAX = Abs. convergence criterion (comp) [ppb]

FLUID PROPERTIES

9

0.000E-0	1.0	0.0	1.000	0.00	0.00
COMPFL	CW	SIGMAW	RHOW0	URHOWO	DRWDU
D10.0	D10.0	D10.0	D10.0	D10.0	D10.0

COMPFL = β $(m \cdot s^2/kg)$ fluid compressibility
CW = C_w [1] specific heat of water (energy)
SIGMAW = D_{sw} $[m^2/S]$ molecular diffusivity of water (solute)
RHOW0 = ρ_o $[kg/m^3]$ density of pure water
URHOWO = C_o $[kg_s/kg_w]$ solute concentration at reference conditions
DRWDU = $d\rho/dC$ $[kg_w^2/L\text{-}kg_s]$ change in solution density with respect to solute concentration

SOLID MATRIX PROPERTIES

10

0.00E0	0.0E0	0.0E0	1.0	1.0		
COMPMA	CS	SIGMAS	RHOS	SWRES	PCENT	PCRES
D10.0	D10.0	D10.0	D10.0	D10.0	D10.0	D10.0

COMPMA = Porous matrix compressibility. (α) [m·sec²/kg]
CS = Matrix Specific Heat, h [Cal/kg-°C]
SIGMAS = Solid grain diffusivity [m²/sec]
RHOS = Solid grain density [kg/m³]
SWRES = Residual saturation [fraction of pore volume]
PCENT = Entry capillary pressure [ ]
PCRES = PC @ SWRES [ ]

SOLUTE DECAY RATE

11

0.0E-9
DECAY
D10.0

DECAY = Radioactive decay constant [1/sec]

COORD ORIENT. TO GRAVITY

12

00.0	00.0
GRAVX	GRAVY
F10.0	F10.0

GRAVX = |g| (dz/dx) [m/s²]
GRAVY = |g| (dz/dy) [m/s²]

SCALE FACTORS FOR NODEWISE DATA

13a

152.4	228.6	30.5	0.20
SCALX	SCALY	SCALTH	PORFAC
F10.0	F10.0	F10.0	F10.0

SCALX = X coordinate scale factor [152.4 m]
SCALY = Y coordinate scale factor [228.6 m]
SCALTH = Thickness scale factor [30.5 m]
PORFAC = Porosity scale factor [0.35]

NODEWISE DATA

	1	0.	0.	1.30	1.00
	2	1.	0.	1.00	1.00
13 B					
	II	X(II)	Y(II)	THICK(II)	POR(II)
	I5	F10.0	F10.0	F10.0	F10.0

II	=	Node index number	[ ]
X(II)	=	X Coordinate	[ ]
Y(II)	=	Y Coordinate	[ ]
THICK(II)	=	Thickness	[ ]
POR(II)	=	Porosity	[ ]

ELEMENT INFORMATION

	6.84E-11	6.84E-11	0.	24.	7.2
14 A	PMAXFA	PMINFA	ANGFAC	DSLFAC	DSTFAC
	D10.0	D10.0	F10.0	F10.0	F10.0

PMAXFA	=	K max. (m^2)	(hydraulic conductivity along the axis of greatest conductivity)
PMINFA	=	K min. (m^2)	(hydraulic conductivity along the axis of lowest conductivity]
ANGFAC	=	σ_{kv} [degrees]	(the angle between the axes of lowest and highest conductivity)
DSLFAC	=	α_L [m]	(longitudinal dispersivity)
DSTFAC	=	α_T [m]	(transverse dispersivity)

ELEMENTWISE DATA

14 b

1	1.0	1.0	1.0	1.0	1.0
2	1.0	1.0	1.0	1.0	1.0
L	PMAX	PMIN	ANGLEX	DISPL(L)	DISPT(L)
I10	D10.0	D10.0	D10.0	D10.0	D10.0

L	=	Element index number	[ ]
PMAX	=	Maximum fractional permeability	[ ]
PMIN	=	Minimum fractional permeability	[ ]
ANGLEX	=	Angle between x-axis and max. perm. axis	[ ]
DISPL(L)	=	Longitudinal dispersivity (fractional)	[ ]
DISPT(L)	=	Transverse dispersivity (fractional)	[ ]

PLOT SET-UP DATA

15 a

-1	8	10	132
IDIREC	NLINPI	NCHAPI	NCHAPL
I5	I5	I5	I5

IDIREC = Orientation of Plot :
-1 = Small plot across page
+1 = Large plot along page

NLINPI = Number of lines/inch
NCHAPI = Number of characters/inch
NCHAPL = Number of characters/line

PRESSURE PLOT SCALING

15 b

1.0	1.0E-2
PBASE	PDIGIT
D13.0	D13.0

PBASE = Plotted pressure value = Pressure/PBASE
PDIGIT = Significant digit multiplier for plotted pressure

CONCENTRATIUON PLOT SCALING (D13.0)

15
c

.001E00	1.0E+1
UBASE	UDIGIT
D13.0	D13.0

UBASE = Plotted concentration value = Concentration/UBASE
UDIGIT = Significant digit multiplier for concentration plot

FLOW SOURCE/SINK DATA

16

1	3.25	0.0
2	3.25	0.0
IQCP	QINC	UINC
I10	D15.0	G15.0

IQCP = Node index number
(<0 implies time dependent)
QINC = Flow rate [kg/s] (+) = source (-) = sink
(Leave blank if time-dependent)
UINC = Temperature or conc. [ppb]
(Leave blank if time-dependent)

PRESSURE BOUNDARY CONDITION DATA

17
a

138	44.7	0.0
139	44.7	0.0
IQPC(IPU)	PBC(IPU)	UINC(IPU)
I6	G20.0	G20.0
		(blank line)

IQPC = Node index number [ ]
PBC = Pressure value (if time dependent) [m]
UBC = Conc. BC value (lv · if time dependent) [ppb]

CONCENTRATION BOUNDARY CONDITION DATA

17
b

IUBC	UBC(IPU)	
I6	D20.0	
		(blank line)

IUBX(IPC) = Index number of conc. BC node [ ]
(< 0) = time dependent
UBC(IPC) = Conc. @ BC (lb_s/lb_w)
(< 0) = time dependent [ppb]

NODE/ELEMENT CONNECTIVITY DATA

18
a

1	1	2	22	23
2	2	3	23	24
LL	$IIN_{LL}1$	$IIN_{LL}2$	$IIN_{LL}3$	$IIN_{LL}4$
I6	I6	I6	I6	I6

LL = Element index number (LL <) if pinch node(s) in element)
$IIN_{LL}1$ = The node index number of one of the corner nodes of element LL (Each four nodes must be listed in counterclockwise order, starting at any corner of element.)

209

PINCH NODE INCIDENCE (optional)

18
b

IEDGE(1)	IEDGE(2)	IEDGE(3)	IEDGE(4)
I6	I6	I6	I6

A card 18b follows a card 18a only when the element contains a pinch onde. Each card 18b has 4 fields, one for a pinch node on each side of the element. In each EIDGE(n) Field:
Enter the index number of the pinch node - it is exists there.
Leave a blank field if no pinch node exists there.

DELX(n) = grid size in X direction : half of the distance between the (n+1)st & (n-1)st nodes [ft]

- maximum array size = 50 elements (or the DELX array must be redimensioned.
- variability :
  - from a programming standpoint, the user is free to vary the block size at will as long as DELX is uniform within each column
  - from a mathematical modeling standpoint, DELX should NOT change by more than a factor of 2 between two adjacent rows, due to inherent stability limitations of the algorithm.

VARIABLE GRID CARD(s) -- DELY

DELY(1)	DELY(2)	DELY(3)	DELY(4)	DELY(5)	DELY(6)	DELY(7)	DELY(8)
750.	750.	750.	750.	750.	750.	750.	750.
750.	750.	750.	750.	750.	750.	750.	750.
750.	750.	750.					
F8.0	F8.0	F8.0	F8.0	F8.0	F8.0	F8.0	F8.0

DELY(n) = grid size in Y direction : half of the distance between the (n+1)st & (n-1)st nodes [ft]

- maximum array size = 50 (or the DELY array can be redimensioned)
- variability :
  - from a programming standpoint, the user is free to vary the block size at will, as long as DELY is uniform within each column
  - from a mathematical modeling standpoint, DELY should NOT change by more than a factor of 2 between two adjacent columns, due to inhernt algorithm stability limitations

INITIAL CONDITIONS OF POLLUTION CARD

X1	DX	Y1	DY	DELP
10.0	2.0	16.0	1.0	91.3
F10.3	F10.3	F10.3	F10.3	F10.3

This card is set up for a pollutant load to be injected, randomly over time, by subroutine GENP(PL). It can produce a rectangular source, a line source, or a point source. Because this subroutine cannot fit hte irregular source geometry, we used another source subroutine for Otis. (This is only one of several subroutines to inject solute into the aquifer.)

As the program currently is (and originally was) written :

- only one source can be specified by this subroutine (unless the source code is modified).
- the program currently reads a line of data at this point in the input data file, and treats it as the "Initial Conditions of Pollution Data," which is input to the subroutine GENP(PL).
- if this card were deleted from the data deck, an execution-time READ error would cause the run to ABEND
- when this subroutine will NOT be used, options would be to :
  - "comment out" the offending source code read statement.
  - set PL = 0.0 on the Initial Conditions of Pollution data card.

X1 = X coordinate of upper left corner of the rectangle where the pollutant enters. [ ]

DX = Length of rectangle that pollutant enters [ ]

Y1 = Y coordinate of upper left corner of rectangle where pollutant enters [ ]

DY = Width of rectangle that pollutant enters [ ]

(The above 4 input parameters must fall within the aquifer).
No default values for X1, Y1 (unless the coordinates (0,0) happen to fall within the aquifer)
Default values for DX = 0, DY = 0.
- A line source if either one = 0
- A point source if both = 0

DELP = The time interval over which the particles are randomly generated. (Not part of subroutine GENP(PL).) [days] [ ]

POLLUTION PARAMETER CARD

PL	MAXP	PM	DISPL	DISPT	EPOR	APOR	RD1	KD	RHO
0.	7500	1.77E0	40.	13.	.35	.35	0.0	0.0	2.63
E8.2	I8	E9.4	E8.2	E8.2	E8.2	E8.2	E8.2	E8.2	E8.2

PL = The total mass of pollutant on a 100% concentration basis, per iteration, in the subroutine GENP(PL). (See preceding card.) (Set PL to an insignificantly low PL in the Otis simulation). [lb]

MAXP = Maximum number of particles allowed in aquifer. [ ]
- . User's Manual suggests 5000, but the Otis simulation results were smoother with 7500.
- . The particle arrays, X( ), Y( ) must be dimensioned appropriately in the source code's COMMON statements.
- . The number of particles present in the aquifer at any given time is proportional to the amount of solute present, and will usually change with time.
- . MAXP may be constrained by computer system limits on core memory per user.
- . If the actual number of particles ≤ MAXP, particles can be added to the aquifer, and PM remains constant.
- . If the actual number of particles > MAXP, the number of particles remains constant, and PM increases.

PM = Particle mass [lb]
- . PM = [total solute present (lb)] / [total # of particles present]
  The value entered is an initial estimate. The programmer may adjust PM during the run as follows:
- . Choose a value which will yield an appropriate number of particles, as constrained by :
  - . precision requirements of the simulation
  - . modeling limitations (on minimum MAXP)
  - . computer limitations (on maximum MAXP)
- . If the total number of solute particles in the aquifer would otherwise increase past MAXP, then PM is increased proportionately, instead, and the number of particles is held constant at MAXP.

DISPL = Longitudinal dispersivity (characteristic length) [ft]
. Each time a particle is moved advectively, an additional random dispersion movement takes place. This movement is proportional to the particle's velocity, to the time increment size, and to DISPL. Longitudinal dispersive movement is aligned with the particle's advective velocity vector. Use the size of inhomogeneities or the distances between inhomogeneities for intial estimate. Adjust by trial and error.

DISPT = Transverse dispersivity (characteristic length) [ft]
. Each time a particle is moved advectively, an additional transverse diffusional movement takes place, perpendicular to the particle's advective velocity vector, and proportional to the time increment and to DISPT.
DISPT = (0.1 to 0.5) * DISPL, and most often,
DISPT = 0.3 * DISPL.

EPOR = Effective porosity [ ]
. The porosity available for diffusion ,after tortuosity and dead-end effects are subtracted out.
Expressed as fractional void volume.
. This affects only the solute balance.
. 0.0 < EPOR < 0.7

APOR = Actual (volumetric) porosity [ ]
. The fractional void volume of the aquifer
[liters of water / liter of saturated aquifer]
. This affects only the solute balance
0.0 < APOR < 0.7 EPOR <= APOR

RD1 = Retardation factor = 1 + RHO*KD/EPOR) = V/V_c [ ]
where :
V is the interstitial velocity of the solvent
Vc is the velocity of a concentration front
. minimum value = 1.00 (no adsorption)
. default value = 1.00 (The program sees RD1 = 0.0, and it sets RD1 = 1.0)

KD = Distribution coefficient of the solute) [ ]
(see Freeze & Cherry, Groundwater)
. default : KD = 0 forces RD1 = 1.00

RHO = Matrix bulk mass density [ ]
- Affects only the retardation factor.
- The value for sand is approximately (2.63)(.65)

SINK LOCATION CARD(s)

I	J	MARK
2	38	1
3	37	1
4	37	1

I3 I3 I3

WHERE :

I = X Coordinate of a Sink [ ]
J = Y Coordinate of a Sink [ ]
MARK = Index number (in sink table) of [ ]
the sink that this sink node is associated with.
Many different "sink nodes" can be associated
with one "sink."

- The sinks specified here pertain only to solute transport.
- The groundwater flow routine handles water sinks as leakages and pumpages, without reference to "sinks."
- Both water and solute particles can move horizontally between nodes in the aquifer.
- Water can leak vertically into or out of any the aquifer at any node.
- However, particles can leak vertically into or out of the aquifer only at nodes is connected to a sink.
- The program will keep track of particles flowing into these sinks.
- Any number of nodes can be connected to any sink.
- The program assumes that any water leaking or pumped from a cell will be at the current solute concentration of that cell, so leakage concentrations are NOT specified.

SOURCE CONCENTRATION CARD(s)

I	J	CONSOR
2	16	0.0
2	17	0.0
2	18	0.0

I3 I3 F14.4

WHERE :

I	=	X coordinate of source node	[ ]
J	=	Y coordinate of source node	[ ]
CONSOR	=	concentration of solute in source fluid	[ppm]

NODE CARD(s) (left portion)

I	J	T1	T2	S1	H	Q	R	RH
1	1	0.0D0	0.0D0	.10E-3	0.	0.0	0.0	0.
1	2	0.0D0	0.0D0	.10E-3	0.	0.0	0.0	0.
1	3	0.0D0	0.0D0	.10E-3	0.	0.0	0.0	0.
1	4	0.0D0	0.0D0	.10E-3	0.	0.0	0.0	0.
1	5	0.0D0	0.0D0	.10E-3	0.	0.0	0.0	0.
		.	.	.	.	.	.	.
		.	.	.	.	.	.	.
		.	.	.	.	.	.	.

I3 I3 E9.3 E9.3 E9.3 F8.2 E10.4 E9.3 F8.2

To use default values for all parameters of a node, delete the mode card. If even one default value of a node must be overridden, all parameter values of a node must be specified on the card.

WHERE :

I	=	X Coordinate of node	[ ]
J	=	Y Coordinate of node	[ ]
T1	=	Transmissivity of node in Y direction (This is just an initial value). Every iteration, during the MIADI procedure, the program calculates T1 & T2 from : T(I,J) = PERM(I,J) * (H(i,j) - BOTT(I,J)) (W.T.) OR T(I,J) = PERM(I,J) * (CH(I,J) - BOTT(I,J)) (Artesian)	[gpd/ft]
T2	=	Transmissivity of node in X direction (See T1)	[gpd/ft]
S1	=	Storage Coefficient of aquifer at node under Artesian conditions	[gal]
H	=	Hydraulic Head at node (initial condition.) During a run, H(i,j) is updated at the start of each time increment.	[ft]
Q	=	Distributed Source/Sink Flow into/out of element	[gal/day]
R	=	Recharge coefficient of aquifer at node	[gal/day/ft]
RH	=	Elevation of Land/Water Surface at node	[ft]
RD	=	Elevation of _____ at node . bottom of stream bed OR . evapotranspiration zone	[ft]

NODE CARD(s) (right portion)

[I]	[J]	CH	SF2	PERM1	PERM2	BOTT
1	1	100.0	0.35	0.0	0.0	-108.0
1	2	100.0	0.35	0.0	0.0	-108.0
1	3	100.0	0.35	0.0	0.0	-108.0
1	4	100.0	0.35	0.0	0.0	-108.0
1	5	100.0	0.35	0.0	0.0	-108.0
		.	.	.	.	.
		.	.	.	.	.
		.	.	.	.	.
I3	I3	F8.2	E9.3	E9.3	F9.3	F8.2

I	=	X Coordinate of node {shown here for clarity only}	
J	=	Y Coordinate of node {actually entered on part A }	
S2	=	Storage coefficient of aquifer, at node, under water table conditions	[gal/ft]
CH	=	Elevation of top of aquifer at node	[ft]
PERM1	=	Aquifer permeability at node (i,j) in Y direction	[gal/day/ft^2]
PERM2	=	Aquifer permeability at node (i,j) in X direction	[gal/day/ft^2]
BOTT	=	Elevation of bottom of aquifer at node	[ft]

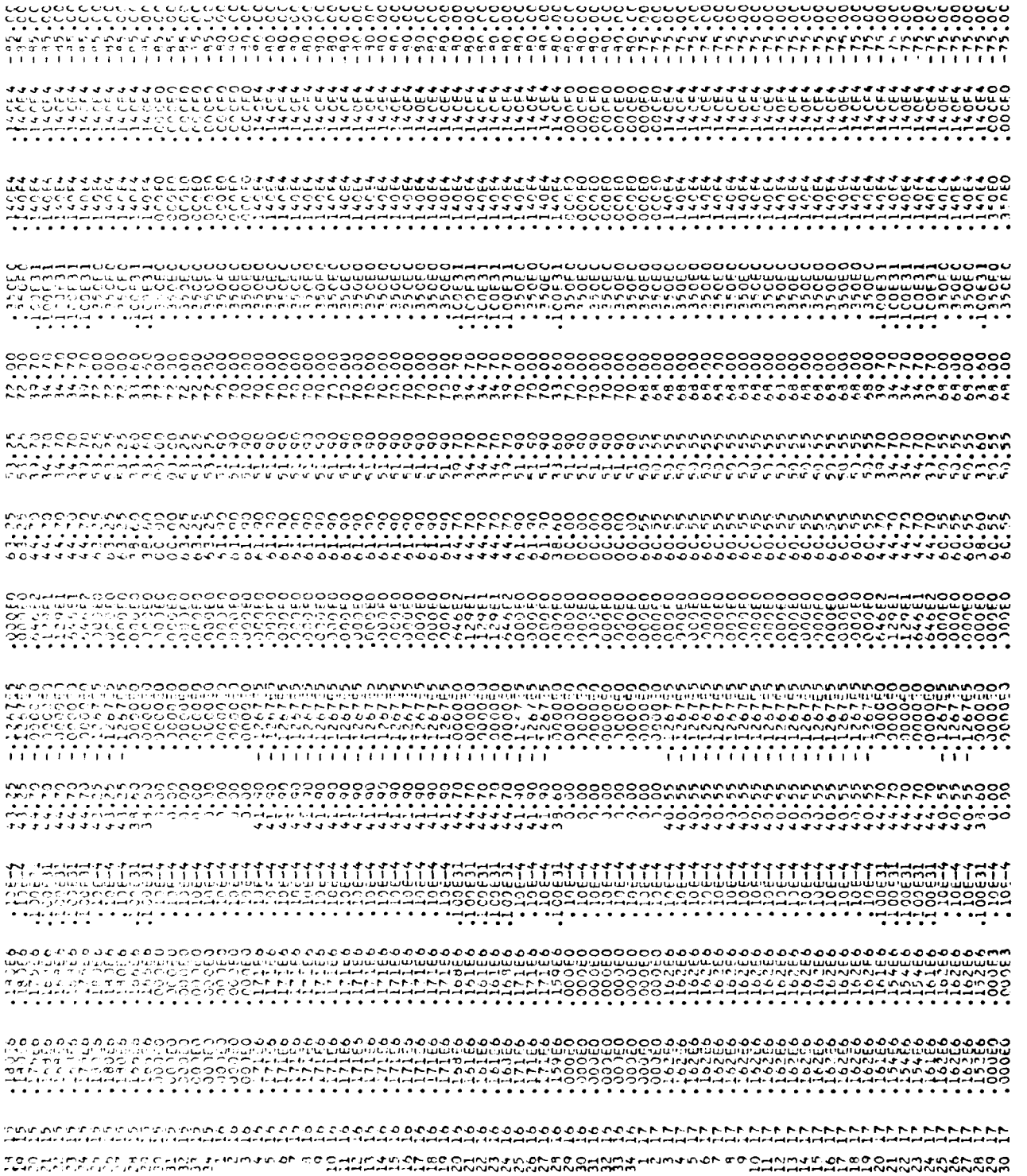
(The reverse of this page is blank.)

APPENDIX F. RANDOM WALK BASE INPUT DATA FILE FOR OTIS SEWAGE PLUME.

```
WHRWOTA   /   ILL R W   /    OTIS ANGR    /   3-31-37   10:05   /    SI = 1.0E-4    /
      1     .10E11  .100E0        40      /  RECH(CH) = 64.6    /  DELTA =   1.0E10  /  MARKS     1 - 4     /
     34        38  .125E6 .125E-3  .40E2   -.13E5    .00E0    .00E0    .0E0   .30E00   .10E2  .140E4  -.14E2
      0         2       1                  /  CP RD = 0.475      /  PM = 1750   L8    /  DEL. PONC NODE (19,15)
 10 10    0.0                             /    4 SW SO ND       /  DISPL = 125.      /  DISPT   =  40.      /
    500.     500.     500.     500.     500.     500.     500.     500.     500.     500.     /  SFI(A) = 1.E30     /
    500.     500.     500.     500.     500.     500.     500.     500.     500.     500.     /  SFI     = 1.E-5     /
    500.     500.     500.     500.     500.     500.     500.     500.     500.     500.     /  NPITS = 40         /
    500.     500.     500.     500.                                                            /  NSP     =  2      /
    750.     750.     750.     750.     750.     750.     750.     750.     750.     750.
    750.     750.     750.     750.     750.     750.     750.     750.     750.     750.
    750.     750.     750.     750.     750.     750.     750.     750.     750.     750.
    750.     750.     750.     750.     750.     750.     750.     750.     750.     750.
       16.          2.          16.          1.      365.25
  .10E1     9000  1.750E3  .125E3   .40E2   .35E0    .35E0     1.00      0.0   2.63E0
  2 38  1
  3 37  1
  4 37  1
  5 39  1
  6 39  1
  7 38  1
  8 38  1
  9 39  1
 10 38  1
 11 38  1
 12 38  1
 13 38  1
 14 39  1
 15 38  1
 16 37  1
 17 37  1
 18 39  1
 19 38  1
 20 37  1
 21 39  1
 22 39  1
 23 38  1
 24 37  1
 25 39  1
 26 38  1
 23 12  2
 21 13  2
 22 13  2
 23 13  2
 20 14  2
 21 14  2
 22 14  2
 23 14  2
 20 15  2
 21 15  2
 22 15  2
 23 15  2
 24 15  2
  9 31  3
  8 32  3
  8 33  3
  7 34  3
  7 35  3
  6 36  3
  6 37  3
  4 20  4
  5 20  4
  4 21  4
  6 21  4
  2 23  4
  3 23  4
  6 22  4
  7 22  4

 16 11  500.0
 15 12  500.0
 16 12  500.0
 17 13  500.0

  1  1  .000E0   .000E0   .10E-4   0.00   .0000E0   .000E0   82.15   72.15   100.00   .350EC   .0C0E0   .C0CF0  -10*.00
  2  1  .000E0   .000E0   .10E-4   0.00   .0000E0   .000E0   82.15   72.15   100.00   .350EC   .0C0E0   .00CF0  -108.CC
  3  1  .000E0   .000E0   .10E-4   0.00   .0000E0   .000E0   82.15   72.15   100.00   .350EC   .0C0E0   .000E0  -108.0C
  4  1  .000E0   .000E0   .10E-4   0.00   .0000E0   .000E0   82.15   72.15   100.00   .350EC   .0C0E0   .00CF0  -108.00
  5  1  .000E0   .000E0   .10E-4   0.00   .0000E0   .000E0   82.15   72.15   100.00   .350EC   .0C0E0   .00CF0  -108.00
  6  1  .000E0   .000E0   .10E-4   0.00   .0000E0   .000E0   82.15   72.15   100.00   .350EC   .0C0E0   .C0CF0  -108.CC
  7  1  .000E0   .000E0   .10E-4   0.00   .0000E0   .000E0   82.15   72.15   100.00   .350EC   .0C0E0   .C0CF0  -108.CC
```



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APPENDIX G

ANNOTATED INPUT DATA FILE TEMPLATE FOR SUTRA 10/82 PROGRAM

Example values for Otis Sewage Plume.

SUTRA	SOLUTE	TRANSPORT
SIMULA (1)	SIMULA (2)	
A6	A6	n(A10)

SIMULA(1) = 'SUTRA '
SIMULA(2) = 'ENERGY' for energy transport problems
= 'SOLUTE' for solute transport problems

Title Card

2

PRELIMINARY INPUT FILE FOR OTIS SEWAGE PLUME 20X24 : SUTRA 2D 10/82 : METRIC UNITS
80A1

TITLE Sufficient information to properly identify the run

Simulation Control Numbers

3

525	480	45	0	87	0	6	+1	0/1	1
NN	NE	NBI	NPINCH	NPBC	NUBC	NSO	ISSTAT	IREAD	ISTORE
I5	I5	I5	I5	I5	I5	I5	I5	I5	I5

NN = Number of Nodes
NE = Number of Elements

NBI = Bandwidth
- find the element with the greatest difference between the highest and lowest node numbers, NNmax and NNmin
- NBI = 2 * (NNmax - NNmin) + 1

NPINCH = Number of Pinch Nodes (nodes NOT located at one of the four 'corners' of a quadrilateral element)

NPBC = Number of Pressure Boundary Conditions.
A node where the pressure is specified over time, and is maintained by a fluid source/sink.

NUBC = Number of Composition/Temperature Boundary Conditions
A node where the temperature/concentration is specified over time, and is maintained by a heat/solute source (or sink)

NSO = Number of (Source & Sink) Node Boundary Conditions

ISSTAT = SS/USS Flow Switch :
SS Flow = 1; USS Flow = 0

IREAD = Hot/Cold Start Switch :
IREAD = 1; Read from Tape 55 cold start
IREAD = 0; Read from TAPE 66 warm start
An efficient way to save and re-start a run that abended due to a power surge, etc. TAPE 66 holds intermediate iteration results. The run can be restarted at the last completed iteration.

ISTORE = Switch to SAVE/drop results of intermediate iterations.
Y = 1; DSBR N ≤ 0, do NOT save

PRESSURE BOUNDARY CONDITION FACTOR

1.00E00
GNUO
D15.0

4

GNUO :
Control the closeness of the specified vs. simulated node pressure match.
Recommended inital value: 0.01. Desired final match: 6-7 signif. fig's.

UPSTREAM WEIGHTING FACTOR

0.00
UP
F10.0

5

UP = Upstream Weighting Factor Range = 0.0 - 1.0
Recommend 0.0 for most problems. (No upstream weighting.)
Higher values (0.5 - 1.0) for highly advective transport or unsaturated flow, where oscillations are a problem.

TEMPORAL CONTROL DATA CARD

6

30	1.57788+7	1.00E10	99	1.00	1	1	10
ITMAX	DELT	TMAX	ITCYC	DTMULT	NPCYC	NUCYC	NPRINT
I10	D10.0	D10.0	I10	F10.0	I10	I10	I10

ITMAX =	Maximum number of time steps	[steps]
DELT =	Initial time step	[sec.]
TMAX =	Maximum simulation time	[sec.]
ITCYC =	Time step change cycle length	[steps]
DTMULT=	Time step change multiplier	[ ]
NPCYC =	Flow solution cycle length	[steps]
NUCYC =	Transport solution cycle length	[steps]
NPRINT=	Printed output cycle	[steps]

OUTPUT CONTROLS AND OPTIONS

7

1	1	1	1	1	1
KCCORD	KELINF	KINCID	KPLOTP	KPLOTU	KVEL
I5	I5	I5	I5	I5	I5

KCOORD	=	Print node coordinate data ?	[1=Y 0=N]
KELINF	=	Print element information (k, α) ?	[1=Y 0=N]
KINCID	=	Print pinch node incidence data set ?	[1=Y 0=N]
KPLOTP	=	Print (LP) pressure plot ?	[1=Y 0=N]
KPLOTU	=	Print (LP) conc/temp plot ?	[1=Y 0=N]
KVEL	=	Print (LP) velocity plot ? (@ elem. centroids)	[1=Y 0=N]

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APPENDIX H

ANNOTATED INPUT DATA FILE TEMPLATE FOR SUTRA 12/84 PROGRAM

CARD #1: Type of Simulation — Read in at line #

SIMULA(1) SIMULA(2)

SUTRA	SOLUTE	TRANSPORT
I6	I6	

Identifies Solute Transport (vs. Heat Transport) Simulations — A1440

SIMULA(1) = "SUTRA" if not, run will abend.
SIMULA(2) = "SOLUTE" for solute transport simulations } affects printout headings, and the handling of numerous input parameters.
= "ENERGY" for energy transport simulations }

normally write " TRANSPORT" in the next 10 spaces, for appearance only.

CARD(S) #2 (a/b): Output Heading (Title) Cards

TITLE

A1820

2 (8A10)

TITLE = up to 2 full lines of text, to clearly identify the run.

CARD #3: Simulation Control Numbers

NN	NE	NBI	NPINCH	NPBC	NUBC	NSOP	NSOU	NOBS	NTOBS
I5	I5	I5	I5	I5	I5	I5	I5	I5	I5

A1860

NN = number of nodes
NE = number of elements

NBI = bandwidth = 2 * (Nmax-Nmin)' + 1
(Nmax - Nmin) = the difference between the largest and smallest node index numbers in an element
(Nmax - Nmin)' = the largest value of (Nmax - Nmin) in the aquifer
NOTE if you haven't done so already, check storage requirements in program lines 75-95.

NPINCH = the number of pinch nodes in the aquifer. No pinch nodes were defined in the Otis simulation.
Until a non-bandwidth-dependent matrix solver is added to the source program, use of pinch nodes will NOT result in major efficiency improvements.

NPBC = the number of pressure bc's specified in the simulation.

NUBC = the number of conc/temp boundary conditions specified in the simulation.

NSOP = the number of fluid source nodes specified in the mesh.

NSOU = the number of U source nodes specified in the mesh.

NOBS = the exact number of nodes at which observations will be made.
Set to 0 for NO observations.

NTOBS = Maximum number of time steps on which observations may be made.
NTOBS ≥ ITMAX/NOBCYC + 1. Set to zero for no observations.

CARD #4: Simulation Node Options

IUNSAT	ISSFLO	ISSTRA	IREAD	ISTORE
I5	I5	I5	I5	I5

IUNSAT = Saturated vs. Unsaturated Flow Switch
0 For unsaturated AND saturated flow
1 For saturated flow ONLY

ISSFLO = Transient vs. Steady-State Groundwater Flow Switch
0 For transient groundwater flow
1 For steady-state groundwater flow

ISSTRA = Transient vs. Steady-State Solute Transport Switch
0 For transient energy or solute transport
1 For steady-state energy or solute transport

IREAD = Cold Start/Warm Start Switch
+1 For Cold Start, taking initial condition data from TAPE55
-1 For Warm Start, taking initial condition data from TAPE66.
Can be used for re-start if the system crashes during the run.

ISTORE = Intermediate Results Storage Switch
- +1 To store the results of the most recently calculated iteration on TAPE66. Normally recommended for longer runs.
- 0 Do NOT store intermediate results directly on TAPE66.

CARD #5: Numerical Control Parameters

UP	GNU
G10.0	G15.0

UP = Weighting Method Switch
0.0 = standard Galerkin method (recommended for most cases)
1.0 = upstream weighting, usually for highly advective cases. This can stop some oscillations. Also increases numerical dispersion.
0.0 - 1.0 User may pick any number in between, as appropriate.

GNU = Pressure boundary condition conductance values
A large value of GNU forces simulated and specified BC values to match very closely. An ideal value of GNU forces a BC match of 6-7 significant figures. GNU Must be found empirically. Suggest initial guess of 0.01.

CARD #6: Temporal Control & Solution Cycling Data

ITMAX	DELT	TMAX	ITCYC	DTMULT	DTMAX	NPCYC	NUCYC
I5	G15.0	G15.0	I10	G10.0	G15.0	I5	I5

ITMAX I5 Maximum allowed number of time steps in simulation.

DELT G15.0 Duration of initial time step. [sec]

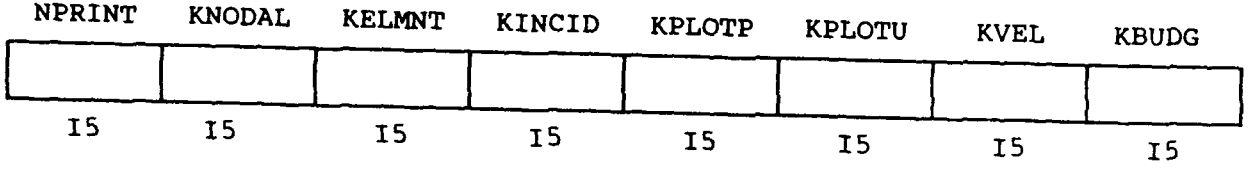
TMAX G15.0 Maximum allowed simulation time. [sec]
(SUTRA time units are always in seconds.)

ITCYC I10 Number of time steps in time step change cycle.
A new time step size is begun at time steps numbered: (1 + N)*(ITCYC).

DTMULT	G10.0	Multiplier for time step change cycle. Next time step size is: (DELT)(DTMULT).
DTMAX	G15.0	Maximum allowed size of time step when using time step multiplier. Time step size is not allowed to increase above this value. [sec]
NPCYC	I5	Number of time steps in pressure solution cycle. Pressure is solved on time steps numbered: N * (NPCYC), as well as on initial time step.
NUCYC	I5	Number of time steps in temperature/concentration solution cycle. Transport equation is solved on time steps numbered: N*(NUCYC) as well as on intial time step.

Either NPCYC or NUCYC must be set to 1.

CARD #7: Output Controls & Options



NPRINT	I5	Printed output is produced on time steps numbered: N*(PRINT), as well as on first and last time steps.
KNODAL	I5	A value of 0 cancels printouts of node coordinates, nodewise element thicknesses, and nodewise porosities. Set to +1 for full printout.
KELMNT	I5	A value of 0 cancels printout of elementwise permeabilities and elementwise dispersivities. Set to +1 for full printout.
KINCID	I5	A value of 0 cancels printout of node incidences and pinch node incidences in elements. Set to +1 for full printout.
KPLOTP	I5	Set to a value of +1 for contourable printer plot of pressures at all nodes in mesh. Set to 0 to cancel pressure plot.
KPLOTU	I5	Set to a value of +1 for contourable printer plot of concentrations or temperatures at all nodes in mesh. Set to 0 to cancel plot.

KVEL I5 Set to a value of +1 to calculate and print fluid velocities at element centroids each time printed output is produced. Note that for non-steady state flow, velocities are based on results and pressures of the previous time step or iteration and not on the newest values. Set to 0 to cancel option.

KBUDG I5 Set to a value of +1 to calculate and print a fluid mass budget and energy or solute mass budget each time printed output is produced. A value of 0 cancels the option.

CARD #8: Iteration Controls

ITRMAX	RPMAX	RUMAX
I10	G10.0	G10.0

ITRMAX I10 Maximum number of iterations allowed per time step to resolve non-linearities. Set to a value of +1 for non-iterative solution. Non-iterative solution may be used for saturated aquifers when density variability of the fluid is small, or for unsaturated aquifers when time steps are chosen to be small.

RPMAX G10.0 Absolute iteration convergence criterion for pressure solution. Pressure solution has converged when largest pressure change from the previous iteration's solution of any node in mesh is less than RPMAX. May be left blank for non-iterative solution. [ ] (1)

RUMAX G10.0 Absolute iteration convergence criterion for transport solution. Transport solution has converged when largest concentration or temperature change from the previous iteration's solution of any node in mesh is less than RUMAX. May be left blank for non-iterative solution. [ ]

CARD #9: Fluid Properities

COMPFL	CW	SIGMAW	RHOWØ	URHOWØ	DRWDU	VISCO
G10.0	G10.0	G10.0	G10.0	G10.0	G10.0	G10.0

(1) Dimensionless.

COMPFL	G10.0	Fluid compressibility, $\beta=(1/\rho)(d\rho/dp)$. . (where ρ = density) $\lvert M/(L\cdot s^2)\rvert^{-1}$. Note, specific pressure storavitity is: $S_{op} = (1-\varepsilon)\alpha + \varepsilon\beta$
CW	G10.0	Fluid specific heat, c_w. $\lvert E/(M\cdot{}^\circ C)\rvert$ (May be left blank for solute transport simulation.)
SIGMAW	G10.0	Fluid diffusivity, σ_w. For energy transport represents fluid thermal conductivity, $\lvert E/(L\cdot{}^\circ C\cdot s)\rvert$. For solute transport represents molecular diffusivity of solute in pure fluid. $\lvert L^2/s\rvert$.
RHOWØ	G10.0	Density of fluid at base concentration or temperature. $\lvert M/L^3\rvert$.
URHWØ	G10.0	Base value of solute concentration (as mass fraction) or temperature of fluid at which base fluid density, RHOWØ is specified. $\lvert M_S/M\rvert$ or $\lvert{}^\circ C\rvert$.
DRWDU	G10.0	Fluid coefficient of density change with concentration (fraction) or temperature: = RHOWØ + DRWDU * (U-URHWØ). $\lvert M/(L^3\cdot M_S)\rvert$ or $\lvert M/(L^3\cdot{}^\circ C)\rvert$
VISCØ	G10.0	For solute transport: fluid viscosity, μ, $\lvert M/L\cdot s\rvert$. For energy transport, this value is a scale factor. It multiplies the viscosity which is calculated internally in units of $\lvert kg/m\cdot s\rvert$. VISC0 may be used for energy transport to convert units of $\lvert kg/m\cdot s\rvert$ to desired units of viscosity.

CAPD #10: Solid Matrix Properties

COMPMA	CS	SIGMAS	RHOS
G10.0	G10.0	G10.0	G10.0

COMPMA	G10.0	Solid matrix compressibility, $\alpha = [1/(1-\varepsilon)] * (d\varepsilon/dp)$. $[M/(L\cdot s^2)]^{-1}$ due mostly to porosity change with pressure.

CS	G10.0	Solid grain specific heat, C_S. [E/(M·°C)] (May be left blank for solute transport simulation.)
SIGMAS	G10.0	Solid grain diffusivity, σ_S. For energy transport represents thermal conductivity of a solid grain. [E/(L·°C·s)] (May be left blank for solute transport simulation.)
RHOS	G10.0	Density of a solid grain, ρ_S. [M/L^3]

CARD #11: Adsorption Parameters

ADSMOD	CHI1	CHI2
A10.0	G10.0	G10.0

ADSMOD	A10	For no sorption or for energy transport simulation write "NONE" beginning in column one, and leave rest of card blank. For linear sorption model, write "LINEAR" beginning in column one. For Freundlich sorption model write "FREUNDLICH" beginning in column one. For Langmuir sorption model write "LANGMUIR" beginning in column one.
CHI1	G10.0	Value of linear, Freundlich or Langmuir distribution coefficient, depending on sorption model chosen as ADSMOD, χ_1. $\lvert L_f^3/M_G \rvert$.
CHI2	G10.0	Value of Freundlich or Langmuir coefficient, depending on sorption model chosen as ADSMOD. Leave blank for linear sorption. χ_2, $\lvert 1 \rvert$ for Freundlich. $\lvert L_f^3/M_S \rvert$ for Langmuir.

CARD #12: Production of Energy or Solute Mass

PRODFO	PRODSO	PRODF1	PRODSI
G10.0	G10.0	G10.0	G10.0

PRODFO	G10.0	Zero-order rate of production in the fluid Γ_o^w. [(E/M)/s] for energy production, [(M_s/M)/s] for solute mass production.
PRODSO	G10.0	Zero-order rate of production in the immobile phase, Γ_o^s. [(E/M_G)/s] for energy production, [(M_s/M_G)/s] for adsorbate mass production.
PRDOF1	G10.0	First-order rate of solute mass production in the fluid, Γ_1^w. [s^{-1}] Leave blank for energy transport.
PRODS1	G10.0	First-order rate of adsorbate mass production in the immobile phase, Γ_1^s. [s^{-1}] Leave blank for energy transport.

CARD #13: Orientation of Coordinates to Gravity

GRAVX	GRAVY
G10.0	G10.0

GRAVX	G10.0	Component of gravity vector in +x direction. [L^2/s] GRAVX = -|g| (d ELEVATION/dx), where |g| is the total acceleration due to gravity in [L^2/s].
GRAVY	G10.0	Component of gravity vector in +y direction. [L^2/s] GRAVY = -|g| (d ELEVATION/dy), where |g| is the total acceleration due to gravity in [L^2/s].

CARD #14: Scale Factor Card for Nodewise Data

SCALX	SCALY	SCALTH	PORFAC
G10.0	G10.0	G10.0	G10.0

	5X	In the first five columns of this card write "NODE", leaving one column blank.

SCALX	G10.0	The scaled x-coordinates of nodes in DATASET 14B are multiplied by SCALX in SUTRA. May be used to change from map to field scales, or from English to SI units. A value of 1.0 gives no scaling. [ ]
SCALY	G10.0	The scaled y-coordinates of nodes in DATASET 14B are multiplied by SCALY in SUTRA. May be used to change from map to field scales, or from English to SI units. A value of 1.0 gives no scaling. [ ]
SCALTH	G10.0	The scaled element (mesh) thicknesses at nodes in DATASET 14B are multiplied by SCALTH in SUTRA. May be used to easily change entire mesh thickness or to convert English to SI units. A value of 1.0 gives no scaling. [ ]
PORFAC	G10.0	The scaled nodewise porosities of DATASET 14B are multiplied by PORFAC in SUTRA. May be used to easily assign a constant porosity value to all nodes by setting PORFAC=porosity, and all POR(II)=1.0 in DATASET 14B. [ ]

CARD #14 B: Nodewise Data

II	X(II)	Y(II)	THICK(II)	POR(II)
1				
2				
3				
4				

II	I5	Number of node to which data on this card refers, ii.
X(II)	G10.0	Scaled x-coordinate of node II, x_{ii}. [L] [ ]
Y(II)	G10.0	Scaled y-coordinate of node II, y_{ii}. [L] [ ]
THICK(II)	G10.0	Scaled thickness of mesh at node II. [L] In order to simulate radial cross-sections, set THICK(II) = $(2\pi)(\text{radius}_{ii})$, where radius_{ii} is the radial distance from the vertical center axis to node ii. [ ]
POR(II)	G10.0	Scaled porosity value at node II, ε_{ii}. [1]

CARD #15 A: Scale Factors for Elementwise Data

---	PMAXFA	PMINFA	ANGFAC	ALMAXF	ALMINF	ATAVGF
10X	G10.0	G10.0	G10.0	G10.0	G10.0	G10.0

	10X	In the first ten columns of this card write "ELEMENT ", leaving three columns blank.
PMAXFA	G10.0	The scaled maximum permeability values of elements in DATASET 15B are multiplied by PMAXFA in SUTRA. May be used to convert units or to aid in assignment of maximum permeability values in elements. [ ]
PMINFA	G10.0	The scaled minimum permeability values of elements in DATASET 15B are multiplied by PMINFA in SUTRA. May be used to convert units or to aid assignment of minimum permeability values in elements. [ ]
ANGFAC	G10.0	The scaled angles between the maximum permeability direction and the x-axis of elements in DATASET 15B are multiplied by ANGFAC in SUTRA. May be used to easily assign a uniform direction of anisotropy by setting ANGFAC= angle, and all ANGLEX(L)=1.0 in DATASET 15B. [ ]
ALMAXF	G10.0	The scaled maximum longitudinal dispersivities of elements in DATASET 15B are multiplied by ALMAXF in SUTRA. May be used to convert units or to aid in assignment of dispersivities. [ ]
ALMINF	G10.0	The scaled minimum longitudinal dispersivities of elements in DATASET 15B are multiplied by ALMINF in SUTRA. May be used to convert units or to aid in assignment of dispersivities. [ ]
ATAVGF	G10.0	The scaled average transverse dispersivities of elements in DATASET 15B are multiplied by ATAVGF in SUTRA. May be used to convert units or to aid in assignment of dispersivity. [ ]

CARD #15B: ELEMENTWISE DATA

L	PMAX(L)	PMIN(L)	ANGLEX(L)	ALMAX(L)	ALMIN(L)	ATAVG(L)
1 2 3 4 5						

L I10 Number of element to which data on this card refers.

PMAX(L) G10.0 Scaled maximum permeability value of element L, $k_{max}(L)$. [L^2]

PMIN(L) G10.0 Scaled minimum permeability value of element L, $k_{min}(L)$. [L^2]
Isotropic permeability requires: PMIN(L)=PMAX(L).

ANGLEX(L) G10.0 Angle measured in counterclockwise direction from +x-direction to maximum permeability direction in element L, Θ_L. [°]
Arbitrary when both PMIN(L)=PMAX(L), and ALMAX(L)=ALMIN(L).

ALMAX(L) G10.0 Scaled longitudinal dispersivity alue of element L in the direction of maximum permeability PMAX(L), $\alpha_{Lmax}(L)$. [L]

ALMIN(L) G10.0 Scaled longitudinal dispersivity value of element L in the direction of minimum permeability PMIN(L), $\alpha_{Lmin}(L)$. [L]

ATAVG(L) G10.0 Scaled average transverse dispersivity value of element L, $\alpha_T(L)$. [L]

CARD #16 - 1: Data for Printer Plot

IDIREC	NLINPI	NCHAPI	NCHAPL
I5	I5	I5	I5

Card 1: (always required when plot is requested)

IDIREC I5 Chooses plot direction:
Set to -1 for small plot, which is oriented across the output page.
Set to +1 for large plot, which is oriented along the output page.

NLINPI I5 Number of printer lines per inch.

NCHAPI I5 Number of printer characters per inch.

NCHAPL I5 Number of printer characters per output line.

The plotting routine prints three digits of each nodal value to be plotted at the (x,y) location of each node on a map of the mesh that the routine constructs. The three digits are not necessarily the first three digits of the value to be plotted, but are always one digit to the left and two digits to the right of the decimal point. Thus, if the value to be plotted is 1234.567, then the digits 456, are printed at the nodal location on the output.

CARD #16 - 2: For Pressure Plots

PBASE

G13.0

PBASE G13.0 Value for scaling plotted pressures.

The pressure value to be plotted, p_{PLOT}, is calculated by SUTRA as $p_{PLOT} = p_i/PBASE$ (p_i = true pressure)
PBASE should be used to scale out powers of ten and to shift the scaled digits of interest to the position of the three plotted digits.

CARD #16 - 3: For Concentration/Temperature Plots

UBASE

G13.0

Card 3: (include this card only when temperature or concentration plots are requested in DATASET 7)

UBASE	G13.0	Value for scaling plotted temperature or concentration values. The value to be plotted, U_{PLOT}, is calculated by SUTRA as: $U_{PLOT} = U_i/UBASE$. (U_i = true value). For example, UBASE may be set to one-tenth of the highest source concentration in the system; then fractional concentrations relative to the highest concentration are plotted with digits ranging from 000 to 999 which represents a relative concentration of 1.000 (≈0.999).

CARD #17 : Data for Fluid Sources/Sinks

IQPC	QIN	UINC
(BLANK)		
I10	G15.0	G10.0

O M I T when there are no fluid source nodes

IQCP	I10	Number of the node to which source/sink data on this card refers. Specifying the node number with a negative sign indicates to SUTRA that the source flow rate and/or the concentration or temperature of the source fluid vary in a specified manner with time. Information regarding a time-dependent source node must be programmed by the user in Subroutine BCTIME, and should not be included on this card.
QINC	G15.0	Fluid source (or sink) which is a specified constant value, QINC, at node IQCP, |M/s| A positive value is a source of fluid to the aquifer. Leave blank if this value is specified as time-dependent in Subroutine BCTIME. Sources are allocated equally by cell among equally sized cells. For unequally sized cells, sources are allocated in proportion to the cell length, area or volume over which the source fluid enters the system.
UINC	G15.0	Temperature or solute concentration (mass fraction) of fluid entering the aquifer. It is a specified constant value for a fluid source at node IQCP, U_{IN}. |°C| or |M_S/M| Leave blank if this value is specified as time-dependent in Subroutine BCTIME.

Last Card:

BLANK CARD — Placed immediately following all NSOP fluid source node cards.

CARD #18: Data for Energy or Pure Solute Sources & Sinks

OMIT when there are no energy or solute source nodes.

IQCU	QUINC
I10	G15.0
(BLANK)	

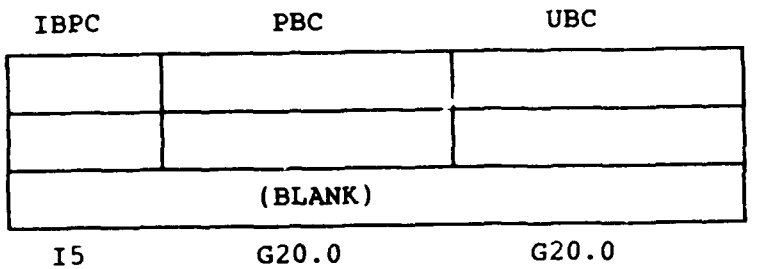
IQCU I10 — Number of the node to which source/sink data on this card refers. Specifying the node number with a negative sign indicates to SUTRA that the source rate varies in a specified manner with time. All information regarding a time-dependent source node must be programmed by the user in Subroutine BCTIME, and a value should not be included in this card.
Sources are allocated equally by cell for equally sized cells. For unequally sized cells, sources are allocated in proportion to the cell length, area or volume over which the source energy or solute mass enters the system.

QUINC G15.0 — Source (or sink) which is a specified constant value, Φ_{in}, at node IQCU. $|E/s|$ for energy transport, $|M_s/s|$ for solute transport. A positive value is a source to the aquifer. Leave blank if IQCU is negative, and this value is specified as time-dependent in Subroutine BCTIME.

Last Card:

BLANK CARD — Placed immediately following all NSOU energy or solute mass source node cards.

CARD #19: Data for Specified Pressure Nodes



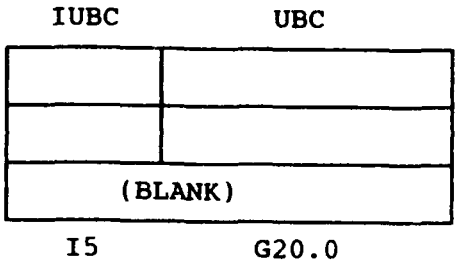
O M I T when there are no specified pressure nodes.

Variable	Format	Description
Cards 1 to NPBC:		
IPBC	I5	Number of the node to which specified pressure data on this card refers. Specifying the node number with a negative sign indicates to SUTRA that the specified pressure value and/or inflow concentration or temperature at this node vary in a specified manner with time. Information regarding a time-dependent specified pressure node must be programmed by the user in Subroutine BCTIME, and should not be included on this card.
PBC	G20.0	Pressure value which is a specified constant at node IPBC. $\lvert M/(L \cdot s^2) \rvert$ Leave blank if this value is specified as time-dependent in Subroutine BCTIME.
UBC	G20.0	Temperature or solute concentration of any external fluid which enters the aquifer at node IPBC. UBC is a specified constant value. $\lvert {}^{\circ}C \rvert$ or $\lvert M_S/M \rvert$ Leave blank if this value is specified as time-dependent in Subroutine BCTIME.

Last Card:

BLANK CARD — Placed immediately following all NPBC specified pressure cards.

CARD #20: Data for Specified Concentration/Temperature Nodes



O M I T when there are no specified concentration or temperature nodes.

Variable	Format	Description
Cards 1 to NUBC:		
IUBC	I5	Number of the node to which specified concentration or temperature data on this card refers. Specifying the node number with a negative sign indicates to SUTRA that the specified value at this node varies in a specified manner with time. This time-dependent value must be programmed by the user in Subroutine BCTIME, and a value should not be included on this card.
UBC	G20.0	Temperature or solute concentration value which is a specified constant at node IUBC.[°C] or [M_s/M]. Leave blank if IUBC is negative and this value is specified as time-dependent in Subroutine BCTIME.

Last Card:

BLANK CARD — Placed immediately following all NUBC specified temperature or concentration cards.

CARD #21: Observation Node Data

NOBCYC

I10

O M I T when there are no observation nodes.

Variable	Format	Description
NOBCYC	I10	Observations of pressure and temperature or concentration will be made at all observation nodes specified below every NOBCYC time steps.

Cards 2 to (NOBS+16)/16

INOB	16I5	Node numbers of observation nodes. (Sixteen nodes per card.) Enter a value of zero as an extra observation node number following the last real observation node in order to indicate to SUTRA that there are no more observation nodes. This will require one extra card if there is an exact multiple of 16 observation nodes.

CARD #22 A: Element Incidence Data

LL	IIN(1)	IIN(2)	IIN(3)	IIN(4)	IIN(5)
1 2 3 4 5					
6 7 8 9 10					

Variable	Format	Description
Card A:	(always required for each element)	
LL	I6	Number of the element to which data on this card (and the optional next card) refers. If pinch nodes exist in element LL, then the element number must be specified with a minus sign.
IIN(1)	I6	Number of node 1
IIN(2)	I6	Number of node 2
IIN(3)	I6	Number of node 3
IIN(4)	I6	Number of node 4

NODE INCIDENCE LIST
List of corner node numbers in element LL, beginning at any corner, but taken in an order counterclockwise about the element.

Card B: (OPTIONAL) - is required immediately following Card A only when LL is negative, O M I T when LL is positive)

PINCH-NODE INCIDENCE LIST

IEDGE(1)	I6	Node number of	IIN(1) and IIN(2)
IEDGE(2)	I6	pinch node at	IIN(2) and IIN(3)
IEDGE(3)	I6	mid-point of edge	IIN(3) and IIN(4)
IEDGE(4)	I6	between nodes:	IIN(4) and IIN(1)

A blank in the list of pinch node numbers indicates that no pinch node exists on that particular edge element LL.

APPENDIX I

SUTRA STORAGE REQUIREMENT CALCULATIONS

TABLE I-1. CALCULATION OF SUTRA-2D-10/82 STORAGE REQUIREMENT FOR A 1-D AQUIFER: MAXIMUM NUMBER OF NODES.

NC_e	= 1	NSOP	= N * 2/65
NR_e	= N	NPBC	= N * 2/65
NN	= 2(N + 1)	NUBC	= N * 2/65
NE	= N	NPINCH	= 0
NBI	= 7	NOBS	= N * 4/65
NNV	= 26	NTOBS	= 10
NEV	= 10	NBCN	= N·4/65

RMDIM = 2*NN * NBI = 2 * 2(N+1) * 7 * 2 = 56 (N + 1)

RVDIM = (NNV * NN) + (NEV * NE) + (NBCN * 4) +

+ (NOBS + 1) * (NTOBS - 2) * 2 + NOBS + NTOBS + 6

= [(26 * 2(N+1)) + (10 * N) + (4 * 4N/65)

+ (1 + .0615N)(10-2)2 + .1538N + 6] * 2

= [52N + 52 + 10N + .25N + 16 + N + .15N + 6]2

= 126.8N + 148

IMVDIM = NE * 8 + NN + NPINCH * 3 + NSOP + NSOU

+ NBCN * 2 + NOBC + NTOBS + 11

= 2[8N + 2N + 2 + 0 + .2n + 11] = 20.4N + 26

RMDIM + RVDIM + IMVDIM = $375{,}000_8$ = 129600 = 203.2N + 230

N = 515.6

For SP: 101.6N = 129,600 - 18700 = 110900

N = 1092

TABLE I-2. CALCULATION OF SUTRA-2D-12/84 STORAGE REQUIREMENTS FOR A 1-D AQUIFER: MAXIMUM NUMBER OF NODES.

$NC_e = 1$

$NR_e = N$

$NN = 2(N + 1)$

$NE = N$

$NBI = 7$

$NNV = 30$

$NEV = 10$

$NSOP = N * 2/65.$

$NPBC = N * 2/65.$

$NUBC = N * 2/65.$

$NPINCH = 0$

$NOBS = N * 4/65.$

$NTOBS = 0$

$NBCN = N * 4/65.$

$RMDIM = 2*NN * NBI = 2* (N+1) * 7 * 2 = 56 (N + 1)$

$RVDIM = ((NNV * NN) + (NEV + 8) * NE + NBCN * 3 +$

$+ (NOBS + 1) * (NTOBS + 2) * 2 + (NTOBS + 5) * 2$

$= [(30(2)(N + 1) + (18)N + .185N$

$(1 + .0615N)(10+2)(2) + 15] * 2$

$= [60N + 60 + 18N + 24 + .185N + 1.5N + 15] * 2$

$= 159.4N + 198$

$IMV = [((NE * 8 + NN + NPINCH * 3 + NSOP +$

$NSOU + NBCN * 2 + NOBC + NTOBS + 12)]2$

$= \{8N + 2N + 2 + 0 + .21*N + 10 + 12)\}2 = 20.4N + 48$

$RMV + RVDIM + IMV = (375,100)_8 = 129600$

$56N + 56 + 159.4N + 198 + 20.4N + 48 = 129600 - 30700$

$235.N = 129298$

$N = 418$

For SP: $117.9N = 106,200$

$N = 901$

TABLE I-3. CALCULATION OF SUTRA-2D-10/82 STORAGE REQUIREMENTS FOR A 2-D AQUIFER: DIMENSIONS OF N * 1.5N NODES.

NC_e	=	NSOP	= 5 * N /225
NR_e	= 1.5 N	NPBC	= 36 * N /225
NN	= (N + 1)(1.5 N + 1)	NUBC	= 0
NE	= 1.5 N + N	NPINCH	= 0
NBI	= N + 2	NOBS	= 5 * N /225
NNV	= 26	NTOBS	= 10
NEV	= 10	NBCN	= 5 * N /225

RMDIM = 2*NN * NBI = 2* (N+1)(1.5N + 1) * (n + 2) * 2

RVDIM = (NNV * NN) + (NEV * NE) + (NBCN * 4) +

+ (NOBS + 1) * (NTOBS - 2) * 2 + NOBS + NTOBS + 6

= (26 * (n + 1)(m + 1)) + (10(n * m))

IMVDIM = NE * 8 + NN + NPINCH * 3 + NSOP + NSOU

+ NBCN * 2 + NOBC + NTOBS + 11

TABLE I-4. PROGRAM LISTING FOR CALCULATION OF DIMENSIONS REQUIRED FOR SUTRA-84 FOR A 2-D RECTANGULAR MESH.

```
100 REM DIMENSIONS REQUIRED FOR SUTRA-84 FOR A 2-D RECTANGULAR MESH
105 REM
110 PRECIS = 2                  ' I             1 = SINGLE PRECISION
120 REM                                         2 = DOUBLE PRECISION
130 NCE = 16                    ' I             NUMBER OF COLUMNS OF ELEMENTS
140 NRE = 20                    ' I             NUMBER OF ROWS OF ELEMENTS
150 NPINCH = 0                  ' I             NUMBER OF PINCH NODES
160 REM                  NCE ≤ NRE
170 NCN = NCE + 1                               '   NUMBER OF COLUMNS OF NODES
180 NRN = NRE + 1                               '   NUMBER OF ROWS OF NODES
190 NN = NCN * NRN                              '   NUMBER OF NODES
200 NE = NCE * NRE                              '   NUMBER OF ELEMENTS
210 NBE = 2 * (NCE + 2) + 1                     '   BANDWIDTH OF MAIN MATRIX
220 NNV = 30                                    '   NUMBER OF VECTORS OF LENGTH ___
230 NEV = 10                                    '   NUMBER OF VECTORS OF LENGTH ___
240 NSOPO = 5                   ' I             '   NUMBER OF NODES WITH P SOURCES
250 NEO = 320                   ' I                 INITIAL NUMBER OF ELEMENTS
260 NSOP = INT(1! * NSOPO * NE / NEO)   '       ADJUSTED FOR NEW MESH DISCRET
270 NSOU0 = 0                   ' I                 NUMBER OF NODES WITH U SOURCES
280 NSOU = INT(1! * NSOU0 * NE / NEO)   '       ADJUSTED FOR NEW MESH DISCRET
290 NPBCO = 25                  ' I                 NUMBER OF NODES WITH P BC
300 NPBC = INT(1! * NPBCO * NE / NEO)   '       ADJUSTED FOR NEW MESH DISCRET
310 NUBCO = 0                   ' I                 NUMBER OF NODES WITH U BC
320 NUBC = INT(1! * NUBCO * NE / NEO)   '       ADJUSTED FOR NEW MESH DISCRET
330 NOBSO = 5                   ' I             NUMBER OF OBSERVATION NODES
340 NOBS = INT(1! * NOBSO * NE / NEO)   '       ADJUSTED FOR NEW MESH DISCRET
350 NTOBS = 10                                  '   PERIOD OF OBSERVATION OUTPUTS
360 NBCN = NPBC + NUBC
370 NRMDIM = 2 * NN * NBI
380 NRMDIM = NRMDIM * PRECIS                    '   ADJUSTED FOR NUMERICAL PRECISION
345 REM
390 NRVDIM = NNV*NN+(NEV+8)*NE+NBCN*3+(NOBS+1)*(NTOBS+2)*2+NTOBS+5
400 REM                                         CORE COMMON STORAGE FOR REAL VECTORS
410 NRVDIM = NRVDIM * PRECIS                    '       ADJUSTED FOR PRECISION
420 IMVDIM = NE*8+NN+NPINCH*3+NSP[+NBCN*2+NSOU+NOBS+NTOBS+11
430 REM                                         CORE COMMON STORAG FOR INTEGER ARRAYS
440 IMVDIM = IMVDIM * PRECIS                    '       ADJUSTED FOR PRECISION
450 NTOT = NRMDIM + NRVCIM + IMVDIM             '   CORE COMMON STORAGE FOR ARRAYS
460 A$="COMMON STORAGE REQUIRED = ": B$="   KILOBYTES DECIMAL"
470 PRINT USING "&";A$
480 PRINT USING"########";NTOT
490 PRINT USING "&";B$
500 D$ = "AVAILABLE CORE MEMORY ON CYBER SYSTEM IS 129.6 K (DECIMAL) AFTER  "
510 PRINT USING "&" ; D$
520 E$ = "         ALLOWING FOR PROGRAM OVERHEAD"
530 PRINT USING "&" ; E$
```

TABLE I-5. PROGRAM LISTING FOR CALCULATION OF DIMENSIONS REQUIRED FOR SUTRA-82 FOR A 2-D RECTANGULAR MESH.

```
100 REM DIMENSIONS REQUIRED FOR SUTRA-82 FOR A 2-D RECTANGULAR MESH
105 REM
110 PRECIS = 2                ' I            1 = SINGLE PRECISION
120 REM                                      2 = DOUBLE PRECISION
130 NCE = 16                  ' I            NUMBER OF COLUMNS OF ELEMENTS
140 NRE = 20                  ' I            NUMBER OF ROWS OF ELEMENTS
145 NPINCH = 0                ' I            NUMBER OF PINCH NODES
150 REM                  NCE ≤ NRE
160 NCN = NCE + 1                            '   NUMBER OF COLUMNS OF NODES
170 NRN = NRE + 1                            '   NUMBER OF ROWS OF NODES
180 NN = NCN * NRN                           '   NUMBER OF NODES
190 NE = NCE * NRE                           '   NUMBER OF ELEMENTS
200 NBE = 2 * (NCE + 2) + 1                  '   BANDWIDTH OF MAIN MATRIX
210 NNV = 26                                 '   NUMBER OF VECTORS OF LENGTH ___
220 NEV = 10                                 '   NUMBER OF VECTORS OF LENGTH ___
230 NSOPO = 5                 ' I            '   NUMBER OF NODES WITH P SOURCES
240 NEO = 320                 ' I                INITIAL NUMBER OF ELEMENTS
250 NSOP = INT(1! * NSOPO * NE / NEO)        '     ADJUSTED FOR NEW MESH DISCRET
260 NSOU0 = 0                 ' I                NUMBER OF NODES WITH U SOURCES
270 NSOU = INT(1! * NSOU0 * NE / NEO)        '     ADJUSTED FOR NEW MESH DISCRET
280 NPBCO = 25                ' I                NUMBER OF NODES WITH P BC
390 NPBC = INT(1! * NPBCO * NE / NEO)        '     ADJUSTED FOR NEW MESH DISCRET
300 NUBCO = 0                 ' I                NUMBER OF NODES WITH U BC
310 NUBC = INT(1! * NUBCO * NE / NEO)        '     ADJUSTED FOR NEW MESH DISCRET
320 NOBSO = 5                 ' I            NUMBER OF OBSERVATION NODES
330 NOBS = INT(1! * NOBSO * NE / NEO)        '     ADJUSTED FOR NEW MESH DISCRET
340 NTOBS = 10                               '   PERIOD OF OBSERVATION OUTPUTS
350 NBCN = NPBC + NUBC
360 NRMDIM = 2 * NN * NBI
370 NRMDIM = NRMDIM * PRECIS                 '   ADJUSTED FOR NUMERICAL PRECISION
345 REM
380 NRVDIM = NNV*NN+NEV*NE+NBCN*4+(NOBS+1)*(NTOBS-2)*2+NOBS+NTOBS+6
390 REM                                    CORE COMMON STORAGE FOR REAL VECTORS
400 NRVDIM = NRVDIM * PRECIS                 '     ADJUSTED FOR PRECISION
410 IMVDIM = NE*8+NN+NSOP+NBCN*2+NPINCH*3+NSOU+NOBS+11
420 REM                                    CORE COMMON STORAG FOR INTEGER ARRAYS
430 IMVDIM = IMVDIM * PRECIS                 '     ADJUSTED FOR PRECISION
440 NTOT = NRMDIM + NRVCIM + IMVDIM          '   CORE COMMON STORAGE FOR ARRAYS
450 A$="COMMON STORAGE REQUIRED = ": B$="   KILOBYTES DECIMAL"
460 PRINT USING "&";A$
470 PRINT USING"########";NTOT
480 PRINT USING "&";B$
490 D$ = "AVAILABLE CORE MEMORY ON CYBER SYSTEM IS 129.6 K (DECIMAL) AFTER  "
500 PRINT USING "&" ; D$
510 E$ = "        ALLOWING FOR PROGRAM OVERHEAD"
520 PRINT USING "&" ; E$
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